

Universal construction for the unsorted quantum search algorithms

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Abstract

The multiple-quantum operator algebra formalism has been exploited to construct generally an unsorted quantum search algorithm. The exponential propagator and its corresponding effective Hamiltonian are constructed explicitly that describe in quantum mechanics the time evolution of a multi-particle two-state quantum system from the initial state to the output of the unsorted quantum search problem. The exponential propagator usually may not be compatible with the mathematical structure and principle of the search problem and hence is not a real quantum search network, but it can be further decomposed into a product of a series of the oracle unitary operations such as the selective phase-shift operations and the nonselective unitary operations which can be expressed further as a sequence of elementary building blocks, i.e., the one-qubit quantum gates and the two-qubit diagonal phase gates, resulting in that the decomposed propagator is compatible with the mathematical structure and principle of the search problem and hence becomes a real quantum search network. The decomposition for the propagator can be achieved with the help of the operator algebra structure and symmetry of the effective Hamiltonian, and the properties of the multiple-quantum operator algebra subspaces, especially the characteristic transformation behavior of the multiple-quantum operators under the z-axis rotations. It has been shown that the computational complexity of the search algorithm is dependent on that of the numerical multidimensional integration and hence it is believed that the search algorithm could solve efficiently the unsorted search problem. An NMR device is also proposed to solve efficiently the unsorted search problem in polynomial time.

1. Introduction

Quantum computation is a cross discipline among mathematics, quantum physics and information science. It obeys both the quantum mechanical laws and the mathematical principles [1-5]. It has been discovered that quantum computers can solve efficiently certain problems in polynomial time that can not be solved efficiently by any classical digital computers [3, 6-11]. The famous examples include the prime factorization [10] and the quantum simulation [3, 11] whose polynomial-time quantum algorithms have been discovered. However, in practice these problems including the prime factorization and the quantum simulation are rather specialized. An important question in quantum computation therefore arises whether or not quantum computers can solve efficiently a general NP problem in polynomial time [10, 12, 13]. It is well known that NP-problems are hard for any classical computation. In the past several years this question has been discussed extensively but has remained largely ignored [12, 13]. On the other hand, it has been found that a quite broad class of problems such as search and optimization problems can be speeded up quadratically by quantum computation [14]. The unsorted search problem is really a hard problem in classical computation. Assume that there is a large unsorted database $T = (0, 1, \dots, N - 1)$ ($N = 2^n$), in which only one of these elements satisfies the function $f(s) = 1$, but $f(r) = 0$ for any other element r ($r \neq s$). Now one wants to find the target element s . If a classical digital computer is used to search for the target element, one will need to examine N elements of the database in the worst case and an average of $N/2$ elements before finding the desired element s . However, Grover [14] has showed recently that if a quantum computer is used one needs to examine only \sqrt{N} elements around to find the target element. It has been proven that the Grover algorithm is the optimal quantum search algorithm so far [15]. Grover and his coworkers has shown further how his search algorithm can speed up quadratically almost any other quantum algorithms [16, 17]. However, the Grover algorithm is not an efficient quantum search algorithm and therefore can not solve efficiently a general NP-problem in polynomial time [12].

One of the most important characteristic features for quantum computation different from classical counterpart is that quantum computers can have the ability of the massive parallel processing in computation [4]. In principle, a quantum computer can offer the possibility for solving efficiently a general NP problem in polynomial time by virtue of the massive quantum

parallelism. However, the quantum computational output usually can not be obtained correctly and directly in polynomial time due to the limits of quantum mechanical measurement. This is the reason why there exists the question whether a quantum computer can solve efficiently a general NP-problem or not. As a consequence of the Grover quantum search algorithm [14], it has been shown that the correct quantum computational output may be obtained after \sqrt{N} iterations and therefore, a general NP problem may be speeded up quadratically by quantum computation [12]. It has been believed extensively that quantum computers can solve efficiently a general NP-problem by virtue of the massive quantum parallelism, although so far only few polynomial-time quantum algorithms have been discovered to solve efficiently some special hard problems [4, 10, 13].

The multiple-quantum operator algebra formalism has been proposed to describe quantum computational process [18, 19]. It has been exploited extensively to design the quantum computational network of a known quantum algorithm [19], construct elementary building blocks of quantum computation [19, 20a], and prepare the effective pure states in the NMR quantum computation [20b]. In this paper the multiple-quantum operator algebra formalism has been used to construct an unsorted quantum search algorithm and its quantum computational networks that obey the quantum mechanical laws and are compatible with the mathematical structure and principles of the unsorted search problem. This quantum search algorithm is different from the Grover's one in that both two algorithms have different propagators. Its computational complexity is dependent on that of the numerical multi-dimensional integration. Therefore, it is believed that the quantum search algorithm could solve efficiently the unsorted search problem on an oracle universal quantum computer. This quantum search algorithm is constructed with two families of elementary unitary operations, that is, the nonselective unitary operations and the oracle unitary operations, e.g., the selective phase-shift operations, all these operations can be further decomposed into a product of a series of elementary building blocks such as one-qubit quantum gates and the two-qubit diagonal phase gates [19]. Here assume that the quantum search algorithm runs on a quantum computer with a quantum system consisting of n two-state particles such as n nuclear spins with the angular momentum quantum number $I=1/2$ and one can manipulate at will each individual two-state particle of the quantum system by an external field such as an electromagnetic field. Also assume that any decoherence effects are ignored in the quantum system.

2. The effective Hamiltonian of a quantum system and the construction of quantum algorithms

Benioff was the first time to use quantum mechanics to describe the reversible computation process on classical Turing machines by understanding the corresponding relationship between the reversible computation process and the fact that time evolution of an isolated quantum system is reversible dynamic [1, 2]. He showed that quantum mechanical models were computationally as powerful as the classical Turing machines. Feynman was the first person to conjecture that quantum mechanical models might be more powerful than any classical computers in simulating quantum processes [3]. His universal quantum simulator could efficiently simulate any quantum dynamics of a quantum system whose Hamiltonian consists of any local interactions [11]. Deutsch formalized the concept of the universal quantum computer and has showed that quantum Turing machines could be more powerful than the classical counterpart from a computational complexity point of view [4]. He has also developed the quantum circuit model of quantum computation [5]. Yao has showed further that the two models of quantum computation, i.e., the quantum Turing machine and the quantum circuit model, are polynomially equivalent to each other [21]. Therefore, there are two ways of thinking about quantum computation [4, 5, 8]. One way is to think of it as the reversible computation on a quantum Turing machine, and another is that quantum computation can be thought of as the unitary time evolution of a quantum system from the input state to the output. The unitary time evolution can be described by a unitary transformation that acts on the input quantum state in a quantum system. In quantum mechanics, time evolution of a quantum system may obey merely quantum mechanical laws, e.g., the Schrödinger equation. Time-evolutional propagator of a quantum system characterizes completely the unitary dynamical behaviors of the quantum system. However, in quantum computation time evolution of a quantum system during quantum computing from the input quantum state to the output is also subjected to the mathematical structure and principle of the problem solved by a given quantum algorithm running on the quantum system in addition to these quantum mechanical laws [19]. Therefore, the form of the propagator is constrained by the mathematical structure and principle of the quantum algorithm. This propagator may be considered generally as a unitary transformation that may be taken as an exponential unitary operator $U(t) = \exp(-iHt)$, where the operator H is the effective Hamil-

tonian of the quantum system subjected to the quantum algorithm. This shows that the form of the effective Hamiltonian H is also constrained by the mathematical structure and principle of the quantum algorithm. Then the effective Hamiltonian H could also really characterize the mathematical structure and properties of the quantum algorithm such as the quantum computational complexity. For example, provided that the effective Hamiltonian H consists of any local interactions in the quantum system, there could be a quantum network that can simulate efficiently time evolution of the quantum system subjected to the quantum algorithm [3, 11]. Obviously, the quantum network is always compatible with the quantum mechanical laws. Is the quantum network also compatible with the mathematical structure and principle of the problem solved by the quantum algorithm? Evidently, if the quantum network is designed according to the mathematical structure and principle of the problem it should be a real quantum computational network to solve the problem, otherwise it can not be thought of as a real quantum network to solve the problem. Now, if the problem solved by the quantum algorithm is an NP-problem this real quantum computational network can solve efficiently the NP-problem because it can simulate efficiently time evolution of the quantum system subjected to the quantum algorithm.

A quantum computation is a unitary time-evolutional dynamical process subjected to a given quantum algorithm from the input quantum states to the output in a quantum system. Now one is given a mathematical problem that needs to be solved on a quantum computer. Assume that there are a number of quantum algorithms to solve the same problem. In practice, one may also design a number of quantum computational networks for a given quantum algorithm to solve the same problem. Consider the special case that the initial state and the output in the quantum system are fixed for a given mathematical problem to be solved on the quantum computer. For example, for the unsorted quantum search problem the initial state is usually considered as the superposition and the output state is the target state in a quantum system. It is well known that there are a number of unitary time-evolutional pathways from the fixed input state to the output in a quantum system. Each such pathway is governed by the quantum mechanical laws and described by a time-evolutional propagator or its corresponding effective Hamiltonian. There may be a unitary dynamical process of the quantum system subjected to the quantum algorithm to solve the problem among all these unitary time-evolutional pathways, and this process is characterized completely by the effective Hamiltonian during running the quantum algo-

rithm. This unitary time-evolutional process obeys not only the quantum mechanical laws but also the mathematical structure and principle of the problem. If there are a number of quantum algorithms to solve the same problem with the fixed input state and the output, there is also a unitary dynamical process corresponding to each such quantum algorithm that obeys both the quantum mechanical laws and the mathematical principles of the problem. Now, assume that the problem is an NP-problem in classical computation, is there an efficient quantum algorithm to solve the problem among these quantum algorithms? If the efficient quantum algorithm exists how to find it and construct its quantum computational network? These problems have not been solved and reminded largely ignored to date. On the other hand, there already exists a simple scheme to find a quantum algorithm to solve a mathematical problem when there is a classical algorithm to solve the same problem. This simple scheme is that a quantum algorithm can be obtained from its corresponding classical algorithm. The computational network of the classical algorithm usually consists of a sequence of irreversible classical logical gates. It can be translated into a quantum algorithm with at least the same computational power by simply replacing the irreversible classical logic gates with the corresponding reversible quantum gates according to the Bennett's suggestion [22]. However, this simple scheme usually may not be available for finding an efficient quantum algorithm to solve a general NP-problem. In this paper the multiple-quantum operator algebra formalism is exploited to design a new quantum algorithm and construct its quantum computational network for a given mathematical problem such as the unsorted search problem [18], where it is assumed that the input state and the output of the quantum system for the problem to be solved are given in advance. Then the total time-evolutional propagator that transforms unitarily the input state to the output can be constructed explicitly. In general, the propagator obeys the quantum mechanical laws but usually is not compatible with the mathematical structure and principle of the problem. Then it is not a real quantum algorithm to solve the problem. However, the propagator may be further decomposed into a sequence of the quantum circuit units which are compatible with the mathematical structure and principle of the problem with the help of the properties of the multiple-quantum operator algebra spaces [18, 19] and the operator algebra structure and symmetry of the effective Hamiltonian. Finally these quantum circuit units are further decomposed into a product of a series of elementary building blocks, i.e., the one-qubit quantum gates and the two-qubit diagonal phase gates [19].

Such constructed quantum network is obviously governed by the quantum mechanical laws and compatible with the mathematical structure and principle of the problem to be solved. Therefore, it becomes a real quantum algorithm to solve the problem. Obviously, once the propagator is decomposed into a product of a polynomial number of elementary building blocks the constructed quantum network is really a polynomial-time quantum computational network to solve efficiently the problem no matter whether the problem is an NP-problem or a polynomial-time problem in classical computation. As an example, a new quantum search algorithm to find the marked element in an unsorted database is explicitly constructed with the help of the multiple-quantum operator algebra formalism. Its quantum computational network consists of the two types of elementary quantum circuit units, that is, the oracle quantum unitary operations, e.g., the selective phase-shift operations, and the nonselective unitary operations, i.e., the oracle-independent quantum unitary operations.

3. The nonselective unitary operations

A nonselective unitary operation is an oracle-independent unitary operation that acts on every two-state particle of a quantum system symmetrically, that is, all the two-state particles in the quantum system are indistinguishable and symmetrical with respect to the unitary operation. The nonselective unitary operations are independent of the marked state to be searched for in the quantum system and can be implemented on a quantum computer without knowing in advance any state of the quantum system. They are also independent of whether the database under search is sorted or unsorted. Therefore, this type of unitary operations are compatible with the mathematical structure and principles of the search problem and can be used to build quantum computational networks of a quantum search algorithm. The Walsh-Hadamard transformation W and the diffusion transform D in the Grover algorithm [14] are typical nonselective unitary operations. Besides the two unitary operations there are a number of other nonselective unitary operations. As an example, two types of general nonselective unitary operations are given below, which may be encountered in present quantum search algorithm. One type of the nonselective rotation operations that are applied to all the two-state particles in a quantum system symmetrically are defined by

$$R_p(\theta, m) = \exp(-i\theta F_p^m) \quad (m = 1, 2, \dots; p = x, y, z). \quad (1)$$

These nonselective unitary operations are constructed with the m th power of

the symmetrical Hermitian operator F_p defined by (in a spin-1/2 language)

$$F_p = \sum_{k=1}^n I_{kp} \quad (2)$$

where the magnetization operator $I_{kp} = \frac{1}{2}\sigma_{kp}$ ($p = x, y, z$), σ_k is the Pauli's operator of the k th two-state particle of the quantum system. Actually, the Walsh-Hadamard transform W can be decomposed into a product of the nonselective unitary operations $R_p(\theta, 1)$ [19]:

$$W = \exp(in\pi/2) \exp(-i\pi F_x) \exp(-i\frac{\pi}{2} F_y). \quad (3)$$

Another type of nonselective unitary operations are defined by

$$T(\theta, \alpha, \beta_x, \beta_y, \beta_z) = \exp(-i\theta \bigotimes_{k=1}^n A_k) \quad (4)$$

where the Hermitian operator A_k of the k th two-state particle of the quantum system may be generally chosen as (in a spin-1/2 language)

$$A_k = \alpha E_k + 2\beta_x I_{kx} + 2\beta_y I_{ky} + 2\beta_z I_{kz} \quad (5)$$

and the parameter vector $\{\beta_p\}$ is a vector with unit magnitude. The real parameters α and β_p ($p = x, y, z$) are independent of any index k , indicating that the unitary operator $T(\theta, \alpha, \beta_x, \beta_y, \beta_z)$ is a nonselective unitary operation. Actually, the nonselective unitary operation can be converted unitarily into simple nonselective phase-shift operations. One of the nonselective phase-shift operations is given by [23, 24]

$$\begin{aligned} C_0(\beta) &= \text{Diag}[e^{-i\beta}, 1, \dots, 1] \\ &= \exp[-i\beta(\frac{1}{2}E_1 + I_{1z}) \otimes (\frac{1}{2}E_2 + I_{2z}) \otimes \dots \otimes (\frac{1}{2}E_n + I_{nz})]. \end{aligned} \quad (6)$$

When $\alpha = 1$ the nonselective unitary operation $T(\theta, \alpha, \beta_x, \beta_y, \beta_z)$ (4) can be transferred into the nonselective phase-shift operation $C_0(\beta)$. Another is defined by

$$S(\beta) = \exp(-i\beta \times 2I_{1z} \otimes 2I_{2z} \otimes \dots \otimes 2I_{nz}). \quad (7)$$

When $\alpha = 0$ the unitary operation $T(\theta, \alpha, \beta_x, \beta_y, \beta_z)$ (4) can be converted unitarily into the nonselective phase-shift operation $S(\beta)$. In particular, the general diffusion transform can be constructed with the nonselective unitary operations mentioned above:

$$D(\theta) = -WC_0(\theta)W. \quad (8)$$

It can prove easily that $D(\theta) = -E + (1 - e^{-i\theta})P$, where E is unity operator and the project operator $P_{ij} = 1/N$, for all i, j . Clearly, the diffusion transform in the Grover algorithm $D = D(\pi)$ [14].

4. The selective unitary transformation and the oracle quantum unitary operation

The selective unitary operations are related only to the marked state $|s\rangle$

that is to be searched for in the quantum system. A type of particularly important selective unitary operations in an unsorted quantum search problem are the selective phase-shift unitary operations. For example, the selective phase inversion operation C_s for the marked state in the Grover search algorithm [14] is a typical selective unitary operation. This type of the selective phase-shift operations can be defined as the diagonal unitary operator $C_s(\theta)$ ($s \neq 0, N-1$) that has diagonal unitary representation in usual quantum computational basis:

$$C_s(\theta) = \text{Diag}\{1, \dots, 1, e^{-i\theta}, 1, \dots, 1\} = \exp[-i\theta E_{ss}] \quad (9)$$

where $[C_s(\theta)]_{ss} = e^{-i\theta}$ only for the diagonal index s , and unit for any other diagonal index $t \neq s$. In particular, the selective phase inversion operation $C_s = C_s(\pi)$ [14]. As an exception, $C_0(\theta)$ and $C_{N-1}(\theta)$ are two nonselective phase-shift operations. The diagonal operator E_{ss} of Eq.(9) can be expressed as

$$E_{ss} = \text{Diag}\{0, \dots, 0, 1, 0, \dots, 0\} \\ = (\frac{1}{2}E_1 + a_1^s I_{1z}) \otimes (\frac{1}{2}E_2 + a_2^s I_{2z}) \otimes \dots \otimes (\frac{1}{2}E_n + a_n^s I_{nz}) \quad (10)$$

where E_k is the 2×2 -dimensional unity operator and $a_k^s = \pm 1$, $k = 1, 2, \dots, n$. It is easy to see that

$$\frac{1}{2}E_k + a_k^s I_{kz} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \text{ if } a_k^s = +1; \frac{1}{2}E_k + a_k^s I_{kz} = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}, \text{ if } a_k^s = -1.$$

When the selective phase-shift operation $C_s(\theta)$ acts on an arbitrary computational basis $|r\rangle$ a phase shift of $\exp(-i\theta)$ is generated if and only if $|r\rangle = |s\rangle$,

$$C_s(\theta)|r\rangle = \exp(-i\theta\delta_{rs})|r\rangle. \quad (11)$$

Obviously, given an n -dimensional unity-number vector $\{a_1^s, a_2^s, \dots, a_n^s\}$ of the marked state $|s\rangle$ the diagonal operator E_{ss} is determined uniquely through Eq.(10) and vice versa. Therefore, the unity-number vector $\{a_1^s, a_2^s, \dots, a_n^s\}$ characterizes completely the diagonal operator E_{ss} and also the selective phase-shift operation $C_s(\theta)$.

In general, a selective phase-shift unitary operation may be defined as a diagonal unitary exponential operator

$$G_s(\theta) = \exp(-i\theta\tilde{H}_s)$$

where the diagonal Hamiltonian $\tilde{H}_s = \tilde{H}_s(a_1^s, a_2^s, \dots, a_n^s)$ is dependent only upon the unity-number vector $\{a_k^s\}$ of the marked state $|s\rangle$. The diagonal Hamiltonian \tilde{H}_s belongs the longitudinal magnetization and spin order (LOMSO) operator subspace of the Liouville operator space of the two-state quantum system and can be generally expressed as a sum of the base operators of the subspace [18]

$$\tilde{H}_s = \Omega'_0 + \sum_{k=1}^n \Omega'_k I_{kz} + \sum_{k < l}^n J'_{kl} 2I_{kz} I_{lz} + \sum_{k < l < m}^n J'_{klm} 4I_{kz} I_{lz} I_{mz} + \dots \quad (12)$$

where all the coefficients $\{\Omega'_k, J'_{kl}, J'_{klm}, \dots\}$ are dependent only on the unity-number vector $\{a_1^s, a_2^s, \dots, a_n^s\}$.

A selective unitary operation is a black-box operation in a quantum search problem because this operation is dependent on the marked state $|s\rangle$, whereas the marked state needs to be searched for in the quantum system. Therefore, the selective unitary operations could be implemented only on an oracle quantum computer. A quantum oracle may be defined as a device that, when called, applies a fixed unitary transformation U_o to the current quantum state $|r\rangle$ of the quantum system, replacing it by $U_o|r\rangle$ [12]. There are some requirements on the unitary transformation U_o in the quantum search problem. The unitary transformation U_o is a selective unitary operation or can be expressed as a sequence of the selective unitary operations and non-selective unitary operations. The effective Hamiltonian of a quantum oracle corresponding to the oracle unitary operation $U_o(\theta) = \exp(-i\theta H_o)$ is therefore expressed as the form

$$H_o = H_o(a_1^s, a_2^s, \dots, a_n^s). \quad (13)$$

Another natural restriction to impose upon U_o may be that U_o is periodic, that is, $U_o^r = E$, r is a known integer, so that the effect of an oracle call can be undone by further $r - 1$ calls, two oracle calls undone by further $r - 2$ calls, and so forth, on the same oracle. The key property of a quantum oracle is its block-box nature [7]. Therefore, an oracle unitary operation could be implemented only on an oracle quantum computer. There are a variety of oracle unitary operations in a quantum search problem. For example, the selective phase inversion operation $C_s(\pi)$ is chosen as an oracle unitary operation in the Grover algorithm whose effective Hamiltonian E_{ss} is given in Eq.(10) and the phase angle $\theta = \pi$ [14]. As a generalization of the selective phase inversion operation $C_s(\pi)$ one can choose conveniently the selective phase-shift operation $C_s(\theta)$ as the oracle unitary operation. The oracle unitary operation $C_s(\theta)$ can be really implemented directly on an oracle universal quantum computer and by using this oracle unitary operation one can construct the unsorted quantum search network, as shown below. Besides the selective phase-shift operation $C_s(\theta)$ the selective unitary operation $U_{op}(\theta) = \exp(-i\theta H_{op})$ whose effective Hamiltonian is given by

$$H_{op} = \sum_{k=1}^n a_k^s I_{kp} \equiv (a_1^s I_{1p}) \otimes E_2 \otimes \dots \otimes E_n \\ + E_1 \otimes (a_2^s I_{2p}) \otimes E_3 \otimes \dots \otimes E_n$$

$$+ \dots + E_1 \otimes \dots \otimes E_{n-1} \otimes (a_n^s I_{np}) \quad (p = x, y, z) \quad (14)$$

also may be a suitable oracle unitary operation used to construct the quantum search network because it may be implemented directly on an NMR quantum computer, as shown in Appendix A and C. The effective Hamiltonian H_{op} is traceless and the selective unitary operation $U_{op}(\theta)$ of the Hamiltonian H_{op} can be expressed as

$$U_{op}(\theta) = \prod_{k=1}^n \exp[-i\theta a_k^s I_{kp}]. \quad (15)$$

Note that the three oracle unitary operations with different $p = x, y, z$ are equivalent to each other by a simple nonselective unitary transformation, for example, $U_{oy}(\theta) = \exp(i\frac{\pi}{2}F_x)U_{oz}(\theta)\exp(-i\frac{\pi}{2}F_x)$ and $U_{ox}(\theta) = \exp(-i\frac{\pi}{2}F_y) \times U_{oz}(\theta)\exp(i\frac{\pi}{2}F_y)$. Obviously, $[U_{op}(\theta)]^r = E$ when $r\theta = 4\pi$. The oracle unitary operation is really single-qubit p -axis pulse applied to all the two-state particles in the quantum system and the phase of the pulse applied to the k th two-state particle is taken as $(-\theta a_k^s)$. It is well known that single-qubit quantum operations are always implemented easily in quantum computation. Therefore, this oracle unitary operation is very simple. By exploiting the oracle unitary operation $U_{op}(\theta)$ one can decomposed the selective phase-shift operation $C_s(\theta)$ into a product of a polynomial number of the oracle unitary operations $U_{op}(\theta)$ and the nonselective unitary operations

$$C_s(\theta) = \exp(-i\frac{\pi}{2}F_y)U_{oy}(-\frac{\pi}{2})C_0(\theta)U_{oy}(\frac{\pi}{2})\exp(i\frac{\pi}{2}F_y). \quad (16)$$

Obviously, if the oracle unitary operation $U_{op}(\theta)$ could be implemented efficiently on an oracle quantum computer the selective phase-shift operation $C_s(\theta)$ could be performed in a polynomial time on the same oracle quantum computer. There is a question whether the oracle unitary operation $U_{op}(\theta)$ can be expressed as a sequence of the selective phase-shift operations $C_s(\theta)$ and the nonselective unitary operations. This question will be discussed in the following section 7.

How to implement the selective phase-shift unitary operation $C_s(\theta)$? Assume that the quantum system is at an arbitrary state including the marked state $|s\rangle$:

$$|\Psi\rangle = |r, S\rangle = \sum_{x=0}^{N-1} a_x |x\rangle [\frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)]$$

where the ancillary qubit S is at the superposition $\frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)$. The evaluation of the function $f(x)$ then can be achieved by performing the oracle unitary operation U_f on the state $|\Psi\rangle$ [12]

$$U_f : |\Psi\rangle \rightarrow \sum_{x=0}^{N-1} a_x |x\rangle [\frac{1}{\sqrt{2}}(|0 \oplus f(x)\rangle - |1 \oplus f(x)\rangle)]$$

$$\begin{aligned}
&= \sum_{x=0}^{N-1} (-1)^{f(x)} a_x |x\rangle \left[\frac{1}{\sqrt{2}} (|0\rangle - |1\rangle) \right] \\
&= \sum_{x=0, x \neq s}^{N-1} a_x |x\rangle \left[\frac{1}{\sqrt{2}} (|0\rangle - |1\rangle) \right] - a_s |s\rangle \left[\frac{1}{\sqrt{2}} (|0\rangle - |1\rangle) \right]
\end{aligned}$$

where the function $f(s) = 1$ and $f(r) = 0$, $r \neq s$. Obviously, only the target state $a_s |s\rangle \left[\frac{1}{\sqrt{2}} (|0\rangle - |1\rangle) \right]$ is inverted and any other state keeps unchanged when performing once evaluation of the function $f(x)$. Therefore, performing once evaluation of the function $f(x)$ is actually equivalent to applying the selective phase-inversion operation $C_s(\pi)$ to the quantum system. The general selective phase-shift operation $C_s(\theta)$ can be achieved by the following oracle unitary operations

$$\begin{aligned}
U_f : \quad |\Psi\rangle &= \sum_{x=0}^{N-1} a_x |x\rangle |0\rangle |1\rangle \rightarrow \sum_{x=0}^{N-1} a_x |x\rangle |0 \oplus f(x)\rangle |1\rangle \\
V(\theta) : \quad &\rightarrow \sum_{x=0}^{N-1} \exp[-i\theta \delta(f(x), 1)] a_x |x\rangle |0 \oplus f(x)\rangle |1\rangle \\
U_f^{-1} : \quad &\rightarrow \sum_{x=0, x \neq s}^{N-1} a_x |x\rangle |0\rangle |1\rangle + \exp(-i\theta) a_s |s\rangle |0\rangle |1\rangle
\end{aligned}$$

where the function $\delta(f(x), 1) = 1$ if $f(x) = 1$; otherwise $\delta(f(x), 1) = 0$, and two ancillary qubits are used in the implementation of the selective phase-shift operation $C_s(\theta)$. Therefore, the oracle unitary operation $C_s(\theta)$ can be expressed as

$$C_s(\theta) = U_f^{-1} V(\theta) U_f \quad (17)$$

where $V(\theta)$ is a conditional phase-shift operation applying only to the two ancillary qubits [10, 25]. Note that $U_f^2 = 1$ the selective phase-shift operation can be also expressed as $C_s(\theta) = U_f V(\theta) U_f$.

5. Construction of quantum search networks

Assume that each usual quantum computational base $|r\rangle$ of the quantum system corresponds one-to-one to an element of the search database, and in particular, the target element is represented by the marked base $|s\rangle$. A usual quantum computational basis can be taken as a Kronecker product of the common eigenbase of the single-particle spin angular momentum operators I_k^2 and I_{kz} in a two-state multiparticle quantum system, for example,

$$|s\rangle = |\alpha\beta\ldots\alpha\rangle = |\alpha\rangle \otimes |\beta\rangle \otimes \ldots \otimes |\alpha\rangle.$$

In the binary representation the eigenbase $|\alpha\rangle, |\beta\rangle$ are denoted briefly as $|0\rangle, |1\rangle$, respectively. In the spinor or vector representation the eigenbase can be expressed as $|\alpha\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and $|\beta\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$. In the unity-number representation $\{a_1^s, a_2^s, \dots, a_n^s\}$ an arbitrary usual computational basis $|s\rangle$ can be expressed

explicitly as

$$|s\rangle = (\frac{1}{2}T_1 + a_1^s S_1) \otimes (\frac{1}{2}T_2 + a_2^s S_2) \otimes \dots \otimes (\frac{1}{2}T_n + a_n^s S_n) \quad (18)$$

where $T_k = |\alpha\rangle_k + |\beta\rangle_k$ and $2S_k = |\alpha\rangle_k - |\beta\rangle_k$. This shows that the unity-number vector $\{a_1^s, a_2^s, \dots, a_n^s\}$ really characterizes completely the usual quantum computational basis $|s\rangle$ and vice versa. Obviously, $\frac{1}{2}T_k + a_k^s S_k = |\alpha\rangle$ if $a_k^s = 1$; $\frac{1}{2}T_k + a_k^s S_k = |\beta\rangle$ if $a_k^s = -1$.

A general quantum search algorithm to find the marked state in the quantum system may be thought of as a unitary time-evolutional process of the quantum system from the initial superposition $|\Psi\rangle$ into the marked state $|s\rangle$

$$U_S : |\Psi\rangle = \frac{1}{\sqrt{N}} \sum_{k=0}^{N-1} |k\rangle \rightarrow |s\rangle \quad (19)$$

where the unitary operator U_S transforms the initial state to the output of the quantum system and may be taken as the quantum computational network of a quantum search algorithm. There are a number of unitary transformations U_S and different unitary transformations U_S may correspond to different quantum search algorithms. In the Grover search algorithm [14] the unitary transformation U_S is taken as a sequence of the $O(\sqrt{N})$ number of the simple unitary transformations: $-WC_0(\pi)WC_s(\pi)$, where the oracle unitary operation is the selective phase-inversion operation $C_s(\pi)$. Therefore, the Grover search algorithm is a quadratically speed-up unsorted quantum search algorithm. Now, a simple unitary transformation U_S is constructed explicitly that is different from the Grover's one and its corresponding effective Hamiltonian is local. First of all, there is a unitary transformation that transforms unitarily the computational basis $|r\rangle$ to the marked state $|s\rangle$

$$U_{rs}|r\rangle = |s\rangle. \quad (20)$$

This unitary transformation U_{rs} may be simply constructed by

$$U_{rs} = E - E_{rr} - E_{ss} + 2I_x^{rs} \quad (21)$$

where E is the unity operator, the operator E_{rs} is defined by

$$(E_{rs})_{ij} = \delta_{ri}\delta_{sj}, \quad (22)$$

and the single-transition operators are defined by [23]

$$I_x^{rs} = \frac{1}{2}(E_{rs} + E_{sr}), \quad I_y^{rs} = \frac{1}{2i}(E_{rs} - E_{sr}), \quad I_z^{rs} = \frac{1}{2}(E_{rr} - E_{ss}).$$

It can prove that the unitary operator U_{rs} can be further expressed as the exponential form [18]

$$U_{rs} = C_s(\pi) \exp(i\pi I_y^{rs}). \quad (23)$$

Therefore, one of the unitary transformations U_S of Eq.(19) may be expressed as

$$U_S = U_{0s}W = C_s(\pi) \exp(i\pi I_y^{0s})W \quad (24)$$

where the following transformation involved in the Walsh-Hadamard opera-

tion W has be introduced [26]

$$W \frac{1}{\sqrt{N}} \sum_{k=0}^{N-1} |k\rangle = |0\rangle. \quad (25)$$

The exponential unitary operator $\exp(i\pi I_y^{rs})$ could be prepared and performed directly on a quantum computer only when the pair quantum computational base $|r\rangle$ and $|s\rangle$ are known in advance. However, the basis state $|s\rangle$ is the marked state that needs to be searched for in a quantum system. Obviously, this operation is not compatible with the mathematical structure and principle of the search problem. Then the unitary transformation U_S of Eq.(24) is not a real quantum search network. In order to construct a real quantum search algorithm one needs to find another unitary transformation that is entirely equivalent to the unitary operation $\exp(i\pi I_y^{0s})$. This unitary transformation is required to be compatible with the mathematical structure and principle of the search problem. Obviously, if the unitary operation $\exp(i\pi I_y^{0s})$ can be expressed as a sequence of the nonselective unitary operations and the selective unitary transformations, i.e., the oracle quantum unitary operations, the unitary transformation U_S of Eq.(24) will be compatible with the mathematical structure and principle of the quantum search problem and hence becomes a real quantum search network. Obviously, this quantum search algorithm is different from the Grover's one that has a different propagator transforming the initial state to the final state of the search problem [17]. In the following it is shown that it is possible to express the unitary operator $\exp(i\pi I_y^{0s})$ as a sequence of the nonselective unitary transformations and the selective unitary operations, and each of these unitary operations can be further expressed as a sequence of one-qubit quantum gates and the two-qubit diagonal phase gates.

Now the single-transition multiple-quantum operator I_y^{rs} is expressed as

$$I_y^{rs} = \frac{1}{2i}(E_{rr}QE_{ss} - E_{ss}QE_{rr}) \quad (26)$$

where the operator Q is defined by the matrix elements $Q_{ij} = 1$ for all indexes i, j , and can be written in the unity-number representation as the form [20b]

$$Q = 2^n (\frac{1}{2}E_1 + I_{1x}) \otimes (\frac{1}{2}E_2 + I_{2x}) \otimes \dots \otimes (\frac{1}{2}E_n + I_{nx}). \quad (27)$$

By exploiting the operators E_{rr} , E_{ss} , and Q in the unity-number representation one obtains that

$$E_{rr}QE_{ss} = \bigotimes_{k=1}^n f_k(a_k^s, a_k^r), \quad (28a)$$

$$E_{ss}QE_{rr} = \bigotimes_{k=1}^n g_k(a_k^s, a_k^r) \quad (28b)$$

where

$$\begin{aligned}
f_k(a_k^s, a_k^r) &= [\frac{1}{4}(1 + a_k^r a_k^s)E_k + \frac{1}{2}(a_k^r + a_k^s)I_{kz} \\
&\quad + \frac{1}{2}(1 - a_k^r a_k^s)I_{kx} + \frac{1}{2}i(a_k^r - a_k^s)I_{ky}], \\
g_k(a_k^s, a_k^r) &= [\frac{1}{4}(1 + a_k^r a_k^s)E_k + \frac{1}{2}(a_k^r + a_k^s)I_{kz} \\
&\quad + \frac{1}{2}(1 - a_k^r a_k^s)I_{kx} - \frac{1}{2}i(a_k^r - a_k^s)I_{ky}].
\end{aligned}$$

In particular, $a_k^r = +1$, $k = 1, 2, \dots, n$ for the case of $|r\rangle = |0\rangle$ and

$$\begin{aligned}
f_k(a_k^s, a_k^0) &= \begin{cases} \frac{1}{2}E_k + I_{kz}, & \text{if } a_k^s = 1 \\ I_k^+, & \text{if } a_k^s = -1 \end{cases}, \\
g_k(a_k^s, a_k^0) &= \begin{cases} \frac{1}{2}E_k + I_{kz}, & \text{if } a_k^s = 1 \\ I_k^-, & \text{if } a_k^s = -1 \end{cases}
\end{aligned}$$

where $I_k^\pm = I_{kx} \pm iI_{ky}$. Then, by inserting Eq.(28) into Eq.(26) the multiple-quantum operator I_y^{0s} can be rewritten generally as

$$\begin{aligned}
I_y^{0s} &= \frac{1}{2i}(I_{m_1}^+ I_{m_2}^+ \dots I_{m_k}^+ \\
&\quad - I_{m_1}^- I_{m_2}^- \dots I_{m_k}^-)(\frac{1}{2}E_{m_{k+1}} + I_{m_{k+1}z}) \dots (\frac{1}{2}E_{m_n} + I_{m_n z})
\end{aligned} \quad (29)$$

where the Kronecker product symbol \otimes and index order are omitted without confusion and here assume that $a_{m_i}^s = -1$, $i = 1, 2, \dots, k$; $a_{m_i}^s = 1$, $i = k+1, \dots, n$; $m_i = 1, 2, \dots, n$. For example,

$$\begin{aligned}
\frac{1}{2i}(I_1^+ I_3^+ - I_1^- I_3^-)(\frac{1}{2}E_2 + I_{2z}) \dots &= \frac{1}{2i}I_1^+ \otimes (\frac{1}{2}E_2 + I_{2z}) \otimes I_3^+ \otimes \dots \\
&\quad - \frac{1}{2i}I_1^- \otimes (\frac{1}{2}E_2 + I_{2z}) \otimes I_3^- \otimes \dots
\end{aligned}$$

Equation (29) shows that the operator I_y^{0s} is a k -order multiple-quantum coherence operator ($0 < k \leq n$) [23]. Now one makes a unitary transformation on the operator I_y^{0s} to convert it into the diagonal operator [20b],

$$UI_y^{0s}U^+ = \frac{1}{2}E_{00} - \frac{1}{2}E_{ss} \quad (30)$$

where the unitary transformation U turns out to be taken as the form

$$U = \exp(-i\frac{\pi}{4} \times 2^n I_{m_1 x} \dots I_{m_k x} I_{m_{k+1} z} \dots I_{m_n z}). \quad (31)$$

This unitary operator can be further expressed as a sequence of nonselective unitary operations and the selective unitary operation $U_{oy}(\pm\frac{\pi}{4})$:

$$U = \exp(-i\frac{\pi}{4}F_y)U_{oy}(-\frac{\pi}{4})\exp(-i\frac{\pi}{4} \times 2^n I_{1z}I_{2z} \dots I_{nz})U_{oy}(\frac{\pi}{4})\exp(i\frac{\pi}{4}F_y). \quad (32)$$

It follows from Eq.(30) that the unitary transformation $\exp(i\pi I_y^{0s})$ can be expressed explicitly as

$$\exp(i\pi I_y^{0s}) = U^+ C_0(-\pi/2) C_s(\pi/2) U \quad (33)$$

where the unitary operation $C_0(\pi/2)$ is a nonselective unitary operation and $C_s(\theta)$ is the selective phase-shift operation. The unitary operator U (and U^+) consists of the selective unitary operation $U_{oy}(\pm\frac{\pi}{4})$ and the nonselective unitary operations $\exp(\pm i\frac{\pi}{4}F_y)$ and $\exp(\pm i\frac{\pi}{4} \times 2^n I_{1z}I_{2z} \dots I_{nz})$, as shown in Eq.(32). Inserting Eq.(33) into Eq.(24) one writes the unitary transformation U_S as the form

$$U_S = C_s(\pi)U^+ C_0(-\pi/2) C_s(\pi/2) U W. \quad (34)$$

Now, is this unitary operator U_S a real quantum search network? Because the selective phase-shift operation $C_s(\theta)$ can be expressed as a simple sequence of the oracle unitary operation $U_{oy}(\pm\frac{\pi}{4})$ and the nonselective unitary operations $\exp(\pm i\frac{\pi}{2}F_y)$ and $C_0(\theta)$, as shown in Eq.(16), the unitary operator U_S consists of the oracle unitary operation $U_{oy}(\pm\frac{\pi}{4})$ in addition to those nonselective unitary operations. Then the quantum network U_S of Eq.(34) will be a real quantum search network only when the oracle unitary operation $U_{oy}(\pm\frac{\pi}{4})$ can be directly implemented on an oracle quantum computer. I will show in Appendix A and C how an NMR device can be exploited to implement directly and efficiently the oracle unitary operation $U_{oy}(\pm\frac{\pi}{4})$, then the quantum network U_S of Eq.(34) becomes a real efficient quantum search network on the NMR device. On the other hand, it has been shown in Eq.(17) in section 4 that the selective phase-shift operation $C_s(\theta)$ can be implemented directly on an oracle universal quantum computer [12, 14]. Then, the quantum network U_S of Eq.(34) will be a real quantum search network when the oracle unitary operation $U_{oy}(\pm\frac{\pi}{4})$ is expressed explicitly as a sequence of the selective phase-shift operations $C_s(\theta)$ and the nonselective unitary operations. Obviously, this real quantum search network U_S (34) is independent of any specific quantum computer such as an NMR quantum computer and consists of the selective phase-shift operations $C_s(\theta)$ and the nonselective unitary operations such as the Walsh-Hadamard transform W , $\exp(\pm i\frac{\pi}{4} \times 2^n I_{1z} I_{2z} \dots I_{nz})$, etc., which can be decomposed further into a product of a polynomial number $O(n)$ of one-qubit quantum gates and the two-qubit diagonal phase gates [19], as can be seen in next sections.

6. The parallel quantum search networks

As shown in next sections, there is a complex expression for the oracle unitary operation $U_{oy}(\theta)$ as the selective phase-shift operations $C_s(\theta)$ and the nonselective unitary operations. There are four oracle unitary operations $U_{oy}(\theta)$ in the quantum network U_S of Eq.(34). Therefore, the present quantum network is quite complicated and is not highly efficient. To simplify it one first expands the unitary operator of Eq.(32) as

$$U = \frac{1}{\sqrt{2}}[E - i \exp(-i\frac{\pi}{2}F_y)U_{oy}(-\frac{\pi}{2})(-1)^n 2^n I_{1z} I_{2z} \dots I_{nz}] \quad (35)$$

where the following operator identity has been introduced

$$\exp(\pm i\pi F_p) = (\pm i)^n 2^n I_{1p} I_{2p} \dots I_{np} \quad (p = x, y, z). \quad (36)$$

With the help of Eq.(35) the quantum network U_S of Eq.(34) can be expanded as

$$U_S = \frac{1}{2}\{U_a W + U_a^\dagger W - (-i)^{n+1} C_s(\pi) U_b C_0(-\frac{\pi}{2}) W$$

$$-(i)^{n+1}C_0(-\frac{\pi}{2})U_b^+W\} \quad (37)$$

where

$$U_a = C_0(-\frac{\pi}{2})C_s(-\frac{\pi}{2}),$$

$$U_b = \exp(-i\pi F_z) \exp(i\frac{\pi}{2}F_y)U_{oy}(\frac{\pi}{2})C_s(\frac{\pi}{2}).$$

Equation (37) shows that the quantum network U_S is the sum of the four unitary transformations: U_aW , U_a^+W , $C_s(\pi)U_bC_0(-\frac{\pi}{2})W$, $C_0(-\frac{\pi}{2})U_b^+W$, indicating that the quantum network U_S could be achieved if one performs in parallelism the four unitary transformations on the same initial superposition, respectively, and then sums up coherently their outputs according to Eq.(37). Obviously, the parallel quantum network of Eq.(37) is more efficient with respect with the one in Eq.(34) because one needs to perform in parallelism only once the oracle unitary operation $U_{oy}(\frac{\pi}{2})$.

7. The transformation between oracle unitary operations

In a quantum search of an unsorted database the selective phase-shift operations $C_s(\theta)$ can be generally implemented directly on an oracle universal quantum computer, as shown in section 4. Therefore, one needs to express any other oracle unitary operations such as the oracle unitary operation $U_{op}(\theta)$ ($p = x, y, z$) in the quantum network U_S of Eq.(34) as a product of a series of the selective phase-shift operations $C_s(\theta)$ and the nonselective unitary operations. Obviously, the quantum network U_S of Eq.(34) is also real quantum search algorithm when the oracle unitary operation $U_{op}(\theta)$ is expressed as a sequence of the selective phase-shift operations $C_s(\theta)$ and the nonselective unitary operations. How to implement directly the oracle unitary operation $U_{op}(\theta)$ through an NMR device in polynomial time is given in Appendix A and C. It is discussed below how to construct the oracle unitary operation $U_{op}(\theta)$ with the selective phase-shift operations $C_s(\theta)$ and the nonselective unitary operations.

Now the diagonal operator E_{ss} of Eq.(10) is expanded as

$$2^n E_{ss} = E + \sum_{k=1}^n (2a_k^s I_{kz}) + \sum_{1=k<l}^n (2a_k^s I_{kz})(2a_l^s I_{lz})$$

$$+ \sum_{1=k<l<m}^n (2a_k^s I_{kz})(2a_l^s I_{lz})(2a_m^s I_{mz}) + \dots \quad (38)$$

By using the following spin-echo sequence [23] the even-body interactions such as $(2a_k^s I_{kz})(2a_l^s I_{lz})$, $(2a_k^s I_{kz})(2a_l^s I_{lz})(2a_m^s I_{mz})(2a_n^s I_{nz})$, etc., on the right-hand of Eq.(38) are cancelled. One therefore has

$$U_{ss} \equiv \exp(-i\theta H_{ss})$$

$$= \exp(-i\theta 2^n E_{ss}) \exp(-i\pi F_y) \exp(i\theta 2^n E_{ss}) \exp(i\pi F_y)$$

$$= \exp[-i2\theta\{\sum_{k=1}^n (2a_k^s I_{kz}) + \sum_{1=k<l<m}^n (2a_k^s I_{kz})(2a_l^s I_{lz})(2a_m^s I_{mz}) + \dots\}] \quad (39)$$

where the effective Hamiltonian H_{ss} is written as

$$\begin{aligned} \theta H_{ss} &= N\theta E_{ss} - \exp(-i\pi F_y) N\theta E_{ss} \exp(i\pi F_y) \\ &= 2\theta\{\sum_{k=1}^n (2a_k^s I_{kz}) + \sum_{1=k<l<m}^n (2a_k^s I_{kz})(2a_l^s I_{lz})(2a_m^s I_{mz}) + \dots\} \end{aligned} \quad (40)$$

where $N = 2^n$. Since one can manipulate at will any individual two-state particle of the quantum system all the interactions involving only the j th two-state particle ($j = 1, 2, \dots, n$) on the right-hand side of Eq.(39) then can be extracted by using the spin-echo sequence:

$$\begin{aligned} U_{sj} &= U_{ss} \exp(-i\pi I_{jy}) U_{ss}^+ \exp(i\pi I_{jy}) \\ &= \exp[-i4\theta(2a_j^s I_{jz})\{1 + \sum_{1=k<l}^n (2a_k^s I_{kz})(2a_l^s I_{lz}) + \dots\}] \end{aligned} \quad (41)$$

where the sums \sum' with prime symbol run over all indexes except the index j . There are only even-body interactions in addition to the unity operator in the bracket $\{\}$ on the right-hand side of Eq.(41). In order to cancel further all these even-body interactions but leave only the unity operator in the bracket $\{\}$ one may first make a simple unitary transformation on the unitary operator U_{sj} to convert all these even-body interactions into multiple-quantum coherence operators and then uses the phase cycling techniques [23, 27] to cancel them (see next sections),

$$\begin{aligned} \exp(-i\theta H_{jQ}) &\equiv \exp(-i\frac{\pi}{2} F_{jy}) U_{sj} \exp(i\frac{\pi}{2} F_{jy}) \\ &= \exp(-i4\theta(2a_j^s I_{jz})\{1 + \sum_{1=k<l}^n (2a_k^s I_{kx})(2a_l^s I_{lx}) \\ &\quad + \sum_{1=k<l<p<q}^n (2a_k^s I_{kx})(2a_l^s I_{lx})(2a_p^s I_{px})(2a_q^s I_{qx}) + \dots\}) \end{aligned} \quad (42)$$

where the effective Hamiltonian H_{jQ} is given by

$$\begin{aligned} \theta H_{jQ} &= \exp(-i\frac{\pi}{2} F_{jy})\{\theta H_{ss} \\ &\quad - \exp(-i\pi I_{jy})\theta H_{ss} \exp(i\pi I_{jy})\} \exp(i\frac{\pi}{2} F_{jy}) \end{aligned} \quad (43)$$

and it satisfies

$$\begin{aligned} \theta H_{jQ} &\equiv \exp(-i\frac{\pi}{2} F_{jy})\{N\theta E_{ss} \\ &\quad - \exp(-i\pi F_y) N\theta E_{ss} \exp(i\pi F_y)\} \exp(i\frac{\pi}{2} F_{jy}) \\ &\quad - \exp(-i\frac{\pi}{2} F_{jy}) \exp(-i\pi I_{jy})\{N\theta E_{ss} \\ &\quad - \exp(-i\pi F_y) N\theta E_{ss} \exp(i\pi F_y)\} \exp(i\pi I_{jy}) \exp(i\frac{\pi}{2} F_{jy}) \\ &= 4\theta(2a_j^s I_{jz})\{1 + \sum_{1=k<l}^n (2a_k^s I_{kx})(2a_l^s I_{lx}) \\ &\quad + \sum_{1=k<l<p<q}^n (2a_k^s I_{kx})(2a_l^s I_{lx})(2a_p^s I_{px})(2a_q^s I_{qx}) + \dots\} \end{aligned} \quad (44)$$

where the operator $F_{jp} = \sum_{k=1, k \neq j}^n I_{kp}$ ($p = x, y, z$). Note that there are the identities for the selective phase-shift operation $C_s(\theta)$:

$$\begin{aligned} C_s(\pm N\theta) &= \exp(\mp i\theta 2^n E_{ss}) \\ &= \exp[\mp i(2^n \theta \bmod(2\pi)) E_{ss}] = C_s(\pm N\theta \bmod(2\pi)). \end{aligned} \quad (45)$$

It follows from Eqs.(41)-(44) that the unitary operator $\exp(-i\theta H_{jq})$ can be expressed explicitly as

$$\begin{aligned} \exp(-i\theta H_{jq}) &= \exp(-i\theta H_{jq}) \\ &= \exp(-i\frac{\pi}{2} F_{jy}) C_s(N\theta \bmod(2\pi)) \exp(-i\pi F_y) C_s(-N\theta \bmod(2\pi)) \\ &\quad \times \exp(-i\pi I_{jy}) C_s(N\theta \bmod(2\pi)) \exp(i\pi F_y) C_s(-N\theta \bmod(2\pi)) \\ &\quad \times \exp(i\pi I_{jy}) \exp(i\frac{\pi}{2} F_{jy}) \end{aligned} \quad (46)$$

where the effective Hamiltonian H_{jq} is written as

$$\begin{aligned} \theta H_{jq} &= \exp(-i\frac{\pi}{2} F_{jy}) \{ N\theta \bmod(2\pi) E_{ss} \\ &\quad - \exp(-i\pi F_y) N\theta \bmod(2\pi) E_{ss} \exp(i\pi F_y) \} \exp(i\frac{\pi}{2} F_{jy}) \\ &\quad - \exp(-i\frac{\pi}{2} F_{jy}) \exp(-i\pi I_{jy}) \{ N\theta \bmod(2\pi) E_{ss} \\ &\quad - \exp(-i\pi F_y) N\theta \bmod(2\pi) E_{ss} \exp(i\pi F_y) \} \exp(i\pi I_{jy}) \exp(i\frac{\pi}{2} F_{jy}). \end{aligned} \quad (47)$$

One can see from Eqs.(44) and (47) that the effective Hamiltonian θH_{jq} is proportional to $N\theta$ but the Hamiltonian θH_{jq} is bounded by the norm $\|\theta H_{jq}\| \leq 8\pi$ for any qubit number n . It is well known that the highest order of multiple-quantum coherence is n for a coupled spin ($I=1/2$) system with n two-state particles [23]. This indicates that the operator H_{jq} of Eq.(44) consists of a variety of multiple-quantum coherence operators whose quantum orders take any values from $-(n-1)$ to $(n-1)$ due to the fact that the operator $(2a_j^s I_{jz})$ in the operator H_{jq} is the *LOMSO* operator, which is also a zero-quantum operator [18]. To cancel all these multiple-quantum coherence operators but leave only the desired term $(2a_j^s I_{jz})$ on the right-hand side of the operator H_{jq} of Eq.(44) the discrete Fourier analysis [28] and the phase cycling technique [23, 27] will be exploited below.

7.1 The discrete Fourier analysis and the phase cycling technique

The phase cycling technique is one of the most useful methods in nuclear magnetic resonance (NMR) spectroscopy [23, 27]. It has been used extensively to select the specific multiple-quantum coherences with the desired quantum order and cancel any other undesired multiple-quantum coherences in the NMR experiments. In principle, the phase cycling technique is based on the discrete Fourier transform [28]. The principle of the phase cycling technique can be outlined below. Consider a coupled spin ($I=1/2$) system with n nuclear spins. The density operator $\rho(t)$ of the system then can be

classified generally according to different quantum order p

$$\rho(t) = \sum_{p=-n}^n \rho^p(t). \quad (48)$$

A p -order quantum coherence has an important characteristic transformation behavior under the z-axis rotations [23, 27]

$$\exp(-i\varphi F_z) \rho^p(t) \exp(i\varphi F_z) = \rho^p(t) \exp(-ip\varphi). \quad (49)$$

That is, a p -order quantum coherence generates a phase shift proportional to its quantum order p under the z-axis rotations. This key property is the base to separate different order quantum coherences, to cancel the undesired order and to select the desired order quantum coherences in a coupled multi-spin ($I=1/2$) system. Now by making a series of the z-axis rotations with systematic increments of the phase angle φ_k on the p -order quantum coherence,

$$\varphi_k = k2\pi/N, \quad k = 0, 1, 2, \dots, N-1,$$

and then summing up all the rotational results one obtains

$$\begin{aligned} \frac{1}{N} \sum_{k=0}^{N-1} \exp(-i\varphi_k F_z) \rho^p(t) \exp(i\varphi_k F_z) \\ = \rho^p(t) \left\{ \frac{1}{N} \sum_{k=0}^{N-1} \exp(-i2\pi pk/N) \right\}. \end{aligned} \quad (50)$$

Note that there is the exponential sum relation in the conventional discrete Fourier transform [28],

$$\frac{1}{N} \sum_{k=0}^{N-1} \exp(-i2\pi pk/N) = \begin{cases} 1, & p = 0 \\ 0, & p \neq 0 \end{cases} \quad (51)$$

where p is an integer and $N > |p|$. One can reduce the sum of Eq.(50) to the form

$$\frac{1}{N} \sum_{k=0}^{N-1} \exp(-i\varphi_k F_z) \rho^p(t) \exp(i\varphi_k F_z) = \begin{cases} \rho^0(t), & p = 0 \\ 0, & p \neq 0 \end{cases} \quad (52)$$

Now applying the phase cycling technique to the density operator of Eq.(48) one obtains with the help of Eq.(52)

$$\frac{1}{N} \sum_{k=0}^{N-1} \exp(-i\varphi_k F_z) \sum_{p=-n}^n \rho^p(t) \exp(i\varphi_k F_z) = \rho^0(t) \quad (53)$$

where $N > n$. Equation (53) shows that by N -step phase cycling systematically only the zero-quantum coherence components ($p = 0$) in the density operator of Eq.(48) keep unchanged but all other nonzero order quantum coherences ($p \neq 0$) are cancelled.

Because the operator H_{jQ} of Eq.(44) consists of multiple-quantum coherences with different quantum orders, by replacing the density operator in Eq.(53) with the operator H_{jQ} and with the help of the phase cycling technique all the p -order quantum coherences ($p \neq 0$) are cancelled in the

operator H_{jQ} and one will obtain only the zero-quantum coherences

$$\frac{1}{N} \sum_{k=0}^{N-1} \exp(-i\varphi_{jk}F_{jz})H_{jQ}\exp(i\varphi_{jk}F_{jz}) = H_{jQ}^0 \quad (54)$$

where $N > n - 1$. Note that the operators $I_{kx} = \frac{1}{2}(I_k^+ + I_k^-)$ and $I_{ky} = \frac{1}{2i}(I_k^+ - I_k^-)$. It turns out easily from Eq.(44) and (54) that the zero-quantum operator H_{jQ}^0 can be expressed explicitly as

$$\begin{aligned} H_{jQ}^0 = 4(2a_j^s I_{jz}) \{ & 1 + \sum'_{k \neq l} J_{k,l} (I_k^+ I_l^-) \\ & + \sum'_{k \neq l \neq p \neq q} J_{kl,pq} (I_k^+ I_l^+ I_p^- I_q^-) + \dots \} \end{aligned} \quad (55)$$

where the coefficients $J_{k,l}$, $J_{kl,pq}$, etc., depend on the unity-number vector $\{a_k^s\}$. The Hermiticity of the operator H_{jQ}^0 shows that the coefficients satisfy $J_{k,l} = J_{l,k}^*$, $J_{kl,pq} = J_{pq,kl}^*$, etc.. Equation (54) shows that by $N = n$ step phase cycling one can cancel all the nonzero-order multiple-quantum coherences in the operator H_{jQ} . However, equations (54) and (55) also show that the zero-quantum coherences in the operator H_{jQ} are not cancelled by the phase cycling technique. Therefore, one needs to cancel further the residual zero-quantum coherences in the zero-quantum operator H_{jQ}^0 so as to obtain the desired longitudinal magnetization term $(2a_j^s I_{jz})$.

7.2 The cancellation for the zero-quantum coherences

There is also the important characteristic transformation behavior under the z-axis rotations applied to each individual spin in a spin system, like Eq.(49) [23],

$$\exp(-i2\pi p f_k I_{kz}) I_k^\pm \exp(i2\pi p f_k I_{kz}) = I_k^\pm \exp(\mp i2\pi p f_k), \quad (56)$$

where f_k is called the offset frequency of the k th spin in the spin system. Note that one can manipulate each individual spin in the system by an external field. By making a series of the z-axis rotations applied to each individual spin on the zero-quantum operator H_{jQ}^0 and then summing up all the rotational results one obtains from Eq.(55) with the help of Eq.(56)

$$\begin{aligned} & \frac{1}{N} \sum_{m=0}^{N-1} \exp[-i(2\pi m/N) \sum_{k=1, k \neq j}^n f_k I_{kz}] H_{jQ}^0 \exp[i(2\pi m/N) \sum_{k=1, k \neq j}^n f_k I_{kz}] = \\ & 4(2a_j^s I_{jz}) \{ 1 + \sum'_{k \neq l} \{ J_{k,l} (I_k^+ I_l^-) \frac{1}{N} \sum_{m=0}^{N-1} \exp[-i(2\pi m/N)(f_k - f_l)] \} \\ & + \sum'_{k \neq l \neq p \neq q} \{ J_{kl,pq} (I_k^+ I_l^+ I_p^- I_q^-) \\ & \times \frac{1}{N} \sum_{m=0}^{N-1} \exp[-i(2\pi m/N)(f_k + f_l - f_p - f_q)] \} + \dots \}. \end{aligned} \quad (57)$$

If all the frequencies of the zero-quantum coherences such as $f_k - f_l$, $f_k + f_l - f_p - f_q$, etc. are taken as nonzero integer, it follows from the exponential sum relation (51) that all the zero-quantum coherences on the right-hand side of Eq.(57) are cancelled exactly, leaving only the desired term $4(2a_j^s I_{jz})$ when the step number N is larger than the maximum zero-quantum frequency in Eq.(57). How to choose explicitly the proper offset frequency set $\{f_1, f_2, \dots, f_n\}$ so that all the zero-quantum coherences in Eq.(57) can be cancelled? The suitable integer set of $\{f_1, f_2, \dots, f_n\}$ should satisfy that (a) all the zero-quantum frequencies such as $f_k - f_l$, $f_k + f_l - f_p - f_q$, etc., take nonzero integers and (b) there is a minimum step number $N < \text{poly}(n)$ that does not divide each zero-quantum frequency. The condition $N < \text{poly}(n)$ ensures that all the zero-quantum coherences in the operator H_{jQ}^0 can be cancelled by the phase cycling of Eq.(57) with a polynomial step number N . It is easy to find an offset frequency set $\{f_k\}$ that satisfies only the condition (a). As an example, all the zero-quantum frequencies take nonzero integers if the offset frequency set $\{f_k\}$ is taken as a super-ascend integer series: $f_k > 0$ and $f_{k+1} > \sum_{l=1}^k f_l$, e.g., $\{f_k\} = \{2^0, 2^1, \dots, 2^{n-1}\}$. However, it may be really difficult to find the minimum step number N so that $N < \text{poly}(n)$ when the condition (a) is met. Without losing generality, assume below that all the zero-quantum frequencies f_{zq} take nonzero values. With the aid of Eq.(56) the following integration identity is constructed similar to the summation of Eq.(57)

$$\begin{aligned}
& \frac{1}{2T} \int_{-T}^T dt \exp[-i2\pi t \sum_{k=1, k \neq j}^n f_k I_{kz}] H_{jQ}^0 \exp[i2\pi t \sum_{k=1, k \neq j}^n f_k I_{kz}] = \\
& 4(2a_j^s I_{jz}) \{1 + \sum_{k \neq l}^n \{J_{k,l}(I_k^+ I_l^-) \frac{1}{2T} \int_{-T}^T dt \exp[-i(2\pi t(f_k - f_l))]\} \\
& + \sum_{k \neq l \neq p \neq q}^n \{J_{kl,pq}(I_k^+ I_l^+ I_p^- I_q^-) \\
& \times \frac{1}{2T} \int_{-T}^T dt \exp[-i2\pi t(f_k + f_l - f_p - f_q)]\} + \dots\}. \tag{58}
\end{aligned}$$

Note that for a sufficiently large positive number T and any nonzero zero-quantum frequency f_{zq} ,

$$\frac{1}{2T} \int_{-T}^T dt \exp(-i2\pi t f_{zq}) = \frac{\sin(2\pi T f_{zq})}{2\pi T f_{zq}} = 0. \tag{59}$$

Inserting Eq.(59) into Eq.(58) and making a variable substitution $t = \lambda T$ one obtains

$$\begin{aligned}
4(2a_j^s I_{jz}) &= \frac{1}{2} \int_0^1 d\lambda \{ \exp[-i2\pi\lambda T \sum_{k=1, k \neq j}^n f_k I_{kz}] \\
&\quad \times H_{jQ}^0 \exp[i2\pi\lambda T \sum_{k=1, k \neq j}^n f_k I_{kz}] \\
&\quad + \exp[i2\pi\lambda T \sum_{k=1, k \neq j}^n f_k I_{kz}] H_{jQ}^0 \exp[-i2\pi\lambda T \sum_{k=1, k \neq j}^n f_k I_{kz}] \}. \quad (60)
\end{aligned}$$

The oracle unitary operation $\exp(-i\theta a_j^s I_{jz})$ can be conveniently expressed as, by inserting the zero-quantum operator H_{jQ}^0 of Eq.(54) into Eq.(60),

$$\begin{aligned}
\exp(-i\theta a_j^s I_{jz}) &= \exp\left\{-i\frac{\theta}{16n} \sum_{k'=0}^{n-1} \exp(-i\varphi_{jk'} F_{jz})(H_{jQ}(T) \right. \\
&\quad \left. + H_{jQ}(-T)) \exp(i\varphi_{jk'} F_{jz})\right\} \quad (61)
\end{aligned}$$

where the Hermitian operator $H_{jQ}(T)$ is written as

$$\begin{aligned}
H_{jQ}(T) &= \int_0^1 d\lambda \{ \exp(-i2\pi\lambda T \sum_{k=1, k \neq j}^n f_k I_{kz}) \\
&\quad \times H_{jQ} \exp(i2\pi\lambda T \sum_{k=1, k \neq j}^n f_k I_{kz}) \} \quad (62)
\end{aligned}$$

with the matrix element of any pair of the conventional computational base $|r\rangle$ and $|t\rangle$:

$$\langle r | H_{jQ}(T) | t \rangle = \int_0^1 d\lambda \langle r | H_{jQ} | t \rangle \exp[-i\lambda T \pi \sum_{k=1, k \neq j}^n (a_k^r - a_k^t) f_k].$$

Obviously, $\langle r | H_{jQ}(T) | t \rangle = \langle r | H_{jQ} | t \rangle$ if the multiple-quantum transition frequency equals zero, that is, $\sum_{k=1, k \neq j}^n (a_k^r - a_k^t) f_k = 0$; otherwise, $\langle r | H_{jQ}(T) | t \rangle =$

0. As assumed previously, the zero-quantum transition frequency $\sum_{k=1, k \neq j}^n (a_k^r - a_k^t) f_k \neq 0$ where the transition of the pair of the computational base $|r\rangle$ and $|t\rangle$ is a zero-quantum transition. Then, $\langle r | H_{jQ}(T) | t \rangle = 0$ for any zero-quantum transition between the base $|r\rangle$ and $|t\rangle$. For convenient discussion, first of all, assume that all multiple-quantum transition frequencies including the zero-quantum transition frequencies take nonzero values. Then the transition frequencies $T[\sum_{k=1, k \neq j}^n (a_k^r - a_k^t) f_k]$ are large numbers, that is, $|Tf_k| \gg 1$, for a sufficiently large number T , indicating that the integral of Eq.(62) contains rapidly oscillating periodic integrand. The conventional numerical integration method may not be available for the type of rapidly oscillating integrals [29, 30]. This one-dimensional rapidly oscillating integral may be first converted into a multiple integral before integrating it numerically and this usually will generate an error of $O(\frac{1}{T})$ [30]. It turns out easily that this error is actually zero for the rapidly oscillating periodic integrand

operator of Eq.(62) when T is a sufficiently large number. Let $y_k = \lambda T f_k$, $k = 1, 2, \dots, n$. The one-dimensional rapidly oscillating periodic integral (62) then is converted exactly into the multiple integral:

$$H_{jQ}(T) = \int_0^1 \dots \int_0^1 dy_1 dy_2 \dots dy_n \{ \exp(-i2\pi \sum_{k=1, k \neq j}^n y_k I_{kz}) \times H_{jQ} \exp(i2\pi \sum_{k=1, k \neq j}^n y_k I_{kz}) \}. \quad (63)$$

In fact, the equal matrix element $[H_{jQ}(T)]_{kl}$ of any pair of the usual computational bases $|k\rangle$ and $|l\rangle$ can be obtained from the multiple integral (63) and from the one-dimensional integral (62), respectively. It easily proves from Eqs.(44) and (62) that the Hermitian operator $H_{jQ}(T)$ is a diagonal operator with the norm $\|H_{jQ}(T)\| = 4$ and commutes with the diagonal unitary operators $\exp(\pm i\varphi_{jk} F_{jz})$. Therefore, equation (61) is reduced to the simple form

$$\exp(-i\theta a_j^s I_{jz}) = \exp\{-i\frac{1}{16}\theta H_{jQ}(T)\} \exp\{-i\frac{1}{16}\theta H_{jQ}(-T)\}. \quad (64)$$

This result shows that in the case that all multiple-quantum (including zero-quantum) transition frequencies take nonzero values the phase cycling in section 7.1 to cancel all the nonzero-order multiple quantum coherences becomes not necessary. There are a number of numerical integration methods to calculate a multiple integral [30-36]. One simple numerical method is Hua-Wang method [31, 32] based on the number theory [37]. The lattice point for the numerical multiple integration is chosen as a real algebraic irrational point $(y_1, y_2, \dots, y_n) = \boldsymbol{\omega} = (\omega_1, \omega_2, \dots, \omega_n)$, where $\{1, \omega_1, \omega_2, \dots, \omega_n\}$ are linearly independent real algebraic numbers over the rationals. Then the multiple integral (63) can be replaced with a discrete summation through the numerical multidimensional integration [31, 32]

$$\begin{aligned} & \int_0^1 \dots \int_0^1 dy_1 dy_2 \dots dy_n G_{jQ}(y_1, y_2, \dots, y_n) \\ &= \frac{1}{(2M+1)^l} \sum_{k=-M \times l}^{M \times l} \Phi(M, l, k) G_{jQ}(k\omega_1, k\omega_2, \dots, k\omega_n) + O(M, l) \end{aligned} \quad (65)$$

where the integrand operator is given by

$$\begin{aligned} & G_{jQ}(y_1, y_2, \dots, y_n) \\ &= \exp(-i2\pi \sum_{k=1, k \neq j}^n y_k I_{kz}) H_{jQ} \exp(i2\pi \sum_{k=1, k \neq j}^n y_k I_{kz}) \end{aligned} \quad (66)$$

with the matrix element of any pair of the computational base $|r\rangle$ and $|t\rangle$:

$$\langle r | G_{jQ}(y_1, y_2, \dots, y_n) | t \rangle = \langle r | H_{jQ} | t \rangle \exp[-i\pi \sum_{k=1, k \neq j}^n (a_k^r - a_k^t) y_k].$$

The integer weight distributions $\Phi(M, l, k)$ in Eq.(65) are determined from

the polynomial identity

$$\left(\sum_{k=-M}^M z^k\right)^l = \sum_{k=-M \times l}^{M \times l} \Phi(M, l, k) z^k, \quad (67)$$

and the error function operator $O(M, l)$ can be derived as [31, 32] (also see Appendix B)

$$\langle r | O(M, l) | t \rangle = \begin{cases} -\langle r | H_{jQ} | t \rangle \left(\frac{\sin[(2M+1)\pi(\mathbf{m}(r, t), \boldsymbol{\omega})]}{(2M+1) \sin[\pi(\mathbf{m}(r, t), \boldsymbol{\omega})]} \right)^l, & r \neq t \\ 0, & r = t \end{cases} \quad (68)$$

where the nonzero integer vector $\mathbf{m}(r, t) = (m_1(r, t), m_2(r, t), \dots, m_n(r, t))$ with $m_k(r, t) = (a_k^r - a_k^t)/2 = -1, 0, +1$; $k = 1, 2, \dots, n$. The inner product between the two vectors $\mathbf{m}(r, t)$ and $\boldsymbol{\omega}$ is defined as $(\mathbf{m}(r, t), \boldsymbol{\omega}) = \sum_{k=1}^n \omega_k m_k(r, t)$.

By using the Chebyshev polynomial of the second kind $U_n(\cos \varphi) = \sin((n+1)\varphi)/\sin(\varphi)$ the error function of Eq.(68) is reduced to the form

$$\langle r | O(M, l) | t \rangle = -\langle r | H_{jQ} | t \rangle \left[\frac{U_{2M}(\cos \varphi)}{(2M+1)} \right]^l, \quad r \neq t \quad (69)$$

where $\left| \frac{U_{2M}(\cos \varphi)}{(2M+1)} \right| \leq 1$, $\varphi = \varphi(r, t) = \pi \langle (\mathbf{m}(r, t), \boldsymbol{\omega}) \rangle$, $\langle x \rangle$ denotes the distance from the real number x to the nearest integer, i.e., $\langle x \rangle = \min(\{x\}, 1 - \{x\})$, and $\{x\}$ is the decimal part of the real x . By Eq.(44) one can prove that $|\langle r | H_{jQ} | t \rangle| = 4$ for any pair of the computational base $|r\rangle$ and $|t\rangle$. Then it follows from Eqs.(68) and (69) that the error function operator $O(M, l)$ of Eq.(65) is bounded by

$$\begin{aligned} \|O(M, l)\| &\leq \left[\sum_{r=0}^{2^n-1} \sum_{t=0}^{2^n-1} |\langle r | O(M, l) | t \rangle|^2 \right]^{1/2} \\ &\leq \frac{4}{(2M+1)^l} \left[\sum_{r,t=0, r \neq t}^{2^n-1} |U_{2M}(\cos \varphi(r, t))|^{2l} \right]^{1/2}. \end{aligned} \quad (70)$$

This error function can be made as small as desired when the real algebraic irrational lattice point $\boldsymbol{\omega}$ and the numbers M and l in the numerical integration (65) are chosen suitably. The explicit estimate for the error upper bound may be achieved with the Hua-Wang numerical method [31, 32]. As shown in Refs.[31-35, 38], for every real algebraic irrational point $\boldsymbol{\omega}$ and a finite positive number $a \geq 1$ there exists a positive constant $b = b(a, \boldsymbol{\omega}) > 0$ dependent only on the vector $\boldsymbol{\omega}$ and the number a such that

$$\langle (\mathbf{m}(r, t), \boldsymbol{\omega}) \rangle \geq b(a, \boldsymbol{\omega}) h(\mathbf{m}(r, t))^{-a} \quad (71)$$

holds for all nonzero integer vectors $\mathbf{m}(r, t)$ (the Schmidt theorem [38]). In the Schmidt theorem (71), the distance of the integer vector $\mathbf{m}(r, t)$ from the origin is defined by $h(\mathbf{m}(r, t)) = \prod_{k=1}^n \max(1, |m_k(r, t)|)$. Therefore, $h(\mathbf{m}(r, t)) = 1$

for any computational base $|r\rangle$ and $|t\rangle$ in the case of the integrand operator of Eq.(66). Note that $|\sin[\pi(\mathbf{m}(r, t), \boldsymbol{\omega})]| \geq 2 \langle \mathbf{m}(r, t), \boldsymbol{\omega} \rangle$ [31-35]. From the inequalities (70) and (71) it follows that the error function operator is bounded by

$$\|O(M, l)\| \leq 4(4^n - 2^n)^{1/2} \left(\frac{1}{2(2M+1)b(a, \boldsymbol{\omega})} \right)^l. \quad (72)$$

By choosing suitably the numbers M and l , for example, $l \sim n$, $2M+1 \sim b(a, \boldsymbol{\omega})^{-1}$, one can get the desired small error function operator $O(M, l)$ in the numerical integration (65). It is believed that the coefficient $b(a, \boldsymbol{\omega}) > 0$ does not decrease exponentially as the dimension size n of the multiple integral (63) since it is dependent only on both the algebraic irrational $\boldsymbol{\omega}$ and the number a [31-35, 38]. As a consequence, the lattice point number $(2M \times l + 1)$ in the numerical integration (65) does not grow exponentially as the dimension size n .

The Schmidt theorem (71) is still too strong for the numerical multiple integration (65), although the integration (65) requires that the Schmidt theorem (71) hold only for all those nonzero integer vectors $\mathbf{m}(r, t)$ that satisfy

$$\mathbf{m}(r, t) \neq 0, h(\mathbf{m}(r, t)) = 1 \quad (73)$$

instead of for all the nonzero integer vectors $\mathbf{m}(r, t)$. In fact, the error upper bounds (70) and (72) are derived under the previous assumption that all the multiple-quantum transition frequencies take nonzero values. This assumption really corresponds to the condition (73). One can weaken the use of the Schmidt theorem (71) in the evaluation of the error function (70) with the help of the phase cycling technique in section 7.1. Provided that the phase cycling is available in Eq.(61), the Schmidt theorem (71) is required to hold only for those nonzero integer vectors $\mathbf{m}(r, t)$ that satisfy

$$\mathbf{m}(r, t) \neq 0, h(\mathbf{m}(r, t)) = 1, \sum_{k=1}^n m_k(r, t) = 0. \quad (74)$$

Obviously, the assumption that all the zero-quantum transition frequencies take nonzero values corresponds to the condition (74). Although those nonzero integer vectors $\mathbf{m}(r, t)$ that do not satisfy the condition (74) can cause a large error on the right-hand side of Eq.(65), the error is of the nonzero-order multiple-quantum coherences and hence can be further cancelled by the phase cycling technique, as shown in section 7.1. Thus, inserting the numerical integration of Eq.(65) into Eq.(61) one obtains

$$\exp(-i\theta a_j^s I_{jz}) = \exp\left\{-i\frac{\theta}{16n} \sum_{k'=0}^{n-1} \exp(-i\varphi_{jk'} F_{jz})\right\}$$

$$\begin{aligned} & \times \sum_{k=-M \times l}^{M \times l} \frac{\Phi(M, l, k)}{(2M+1)^l} [G_{jQ}(k\omega_1, k\omega_2, \dots, k\omega_n) \\ & + G_{jQ}(-k\omega_1, -k\omega_2, \dots, -k\omega_n)] \exp(i\varphi_{jk'} F_{jz}) - iO_0(M, l) \} \end{aligned} \quad (75)$$

where the error function operator is given by

$$O_0(M, l) = \frac{\theta}{8n} \sum_{k'=0}^{n-1} \exp(-i\varphi_{jk'} F_{jz}) O(M, l) \exp(i\varphi_{jk'} F_{jz}) \quad (76)$$

with the error function operator $O(M, l)$ given by Eq.(68) or (69). Obviously, $\langle r|O_0(M, l)|t \rangle = 0$ for all the nonzero integer vectors $m(r, t)$ that do not satisfy the condition (74). Therefore, one has

$$\langle r|O_0(M, l)|t \rangle = \begin{cases} \frac{\theta}{8} \langle r|O(M, l)|t \rangle, & \text{the conditions (74) hold} \\ 0, & \text{otherwise} \end{cases} \quad (77)$$

and the error upper bound is derived as

$$\|O_0(M, l)\| \leq \frac{4}{(2M+1)^l} \left[\sum'_{r,t=0, r \neq t}^{2^n-1} |U_{2M}(\cos \varphi(r, t))|^{2l} \right]^{1/2} \quad (78a)$$

where the sums run only over all pair of the computational base $|r\rangle$ and $|t\rangle$ of the zero-quantum transition. It follows from (68)-(71) and Eq.(77) that the error function operator $O_0(M, l)$ has the explicit upper bound:

$$\|O_0(M, l)\| \leq \frac{1}{2} |\theta| \left(\binom{2n}{n} - 2^n \right)^{1/2} \left(\frac{1}{2(2M+1)b(a, \omega)} \right)^l \quad (78b)$$

because number of all the linearly independent zero-quantum coherences in the quantum system with n two-state particles is given by [23]

$$Z_0 = \left(\binom{2n}{n} - 2^n \right).$$

Obviously, the error upper bound $\|O_0(M, l)\|$ is much smaller than $\|O(M, l)\|$.

How to express the exponential operator on the right-hand side of Eq.(64) or Eq.(75) as a sequence of the nonselective unitary operations and the selective phase-shift unitary operations? Choose suitably the algebraic irrational point ω and the numbers M and l so that the error $O_0(M, l)$ in Eq.(75) can be neglected. Then the Trotter-Suzuki theory [39-41] is exploited to decompose the exponential operator of Eq.(75) into a sequence of the these unitary operations.

For simplicity, the unitary operation $\exp(-i\theta a_j^s I_{jz})$ of Eq.(75) is rewritten as

$$\begin{aligned} \exp(-i\theta a_j^s I_{jz}) &= \exp\left\{-it \sum_{k'=0}^{n-1} \sum_{k=-M \times l}^{M \times l} A_j(k, k', \omega)\right\} \\ &\times \exp\left\{-it \sum_{k'=0}^{n-1} \sum_{k=-M \times l}^{M \times l} A_j(k, k', -\omega)\right\} + O_0(M, l) \end{aligned} \quad (79)$$

where $t = \theta/2$ due to the fact that $\|2a_j^s I_{jz}\| = 1$, and the Hermitian operator

$A_j(k, k', \omega)$ is written as

$$A_j(k, k', \omega) = \frac{\Phi(M, l, k)}{8n(2M+1)^l} \exp(-i\varphi_{jk'} F_{jz}) \times G_{jQ}(k\omega_1, k\omega_2, \dots, k\omega_n) \exp(i\varphi_{jk'} F_{jz}). \quad (80)$$

With the help of the generalized Trotter formula [39] the unitary operation $\exp(-i\theta a_j^s I_{jz})$ of Eq.(79) can be decomposed approximately as

$$\exp(-i\theta a_j^s I_{jz}) = \left\{ \prod_{k'=0}^{n-1} \prod_{k=-M \times l}^{M \times l} \exp[-it A_j(k, k', \omega)/L_0] \right\}^{L_0} \times \left\{ \prod_{k'=0}^{n-1} \prod_{k=-M \times l}^{M \times l} \exp[-it A_j(k, k', -\omega)/L_0] \right\}^{L_0} + O_0(M, l) + O(L_0) \quad (81)$$

where the error function operator $O(L_0)$ has the upper bound [11]:

$$\left\| L_0 [\exp(-i\theta a_j^s I_{jz}/L_0) - 1 + i\theta a_j^s I_{jz}/L_0] \right\|,$$

and by Eq.(80) the unitary operator $\exp[-itp A_j(k, k', \omega)]$ with any real constant p can be explicitly expressed as

$$\exp[-itp A_j(k, k', \omega)] = \exp(-i\varphi_{jk'} F_{jz}) \times \exp[-itp \frac{\Phi(M, l, k)}{8n(2M+1)^l} G_{jQ}(k\omega_1, k\omega_2, \dots, k\omega_n)] \exp(i\varphi_{jk'} F_{jz}). \quad (82)$$

The number of the unitary operations $\exp[-it A_j(k, k', \omega)/L_0]$ in Eq.(81) are $2L_0 n(2M \times l + 1)$. It follows from Eq.(81) that the oracle unitary operation $U_{oz}(\theta)$ is written as

$$U_{oz}(\theta) = \prod_{j=1}^n \exp[-i\theta a_j^s I_{jz}] = \prod_{j=1}^n \left\{ \prod_{k'=0}^{n-1} \prod_{k=-M \times l}^{M \times l} \exp[-it A_j(k, k', \omega)/L_0] \right\}^{L_0} \times \left\{ \prod_{k'=0}^{n-1} \prod_{k=-M \times l}^{M \times l} \exp[-it A_j(k, k', -\omega)/L_0] \right\}^{L_0} + nO_0(M, l) + nO(L_0) \quad (83)$$

where the error function operator $nO(L_0)$ is less than the upper bound [11]:

$$\max_{j=1}^n \left\{ \left\| nL_0 [\exp(-i\theta a_j^s I_{jz}/L_0) - 1 + i\theta a_j^s I_{jz}/L_0] \right\| \right\}.$$

This error function can be made as small as desired when L_0 is taken as a sufficiently large number, ensuring that the oracle unitary operation $U_{oz}(\theta)$ can be expressed correctly as a sequence of the unitary operations $\exp[-it A_j(k, k', \omega)/L_0]$ as Eq.(83) within the desired small error (here the error $nO_0(M, l)$ can be neglected, see Eq.(78b)). Note that $U_{oy}(\theta) = \exp(i\frac{\pi}{2} F_x) U_{oz}(\theta) \exp(-i\frac{\pi}{2} F_x)$. By inserting the oracle unitary operation $U_{oz}(\theta)$ ($\theta = \pi/4$) of Eq.(83) into Eq.(34) one obtains finally the real quantum search network U_S (34) which is expressed as a sequence of the nonselective unitary operations and the selective phase-shift unitary operations $C_s(\theta)$.

In fact, the decomposition (81) for the unitary operation $\exp(-i\theta a_j^s I_{jz})$ is the first-order approximated decomposition. A more accurate decomposition, that is, the higher order approximated decomposition, may be achieved with the help of the Suzuki theory [39-41]. As suggested by Suzuki [39-41], the exponential operators on the right-hand side of Eq.(79) is first decomposed approximately into a symmetric sequence of simple exponential operators $\exp[-itpA_j(k, k', \omega)]$ ($|p| < 1$) with the error of order $O(t^{2m})$

$$\exp\{-it \sum_{k'=0}^{n-1} \sum_{k=-M \times l}^{M \times l} A_j(k, k', \omega)\} = f_{2m-1}(\{A_j(k, k', \omega)\}) + O(t^{2m}). \quad (84)$$

The $(2m-1)$ -order approximated symmetrized decomposition f_{2m-1} in Eq.(84) can be constructed as

$$f_{2m-1}(\{A_j(k, k', \omega)\}) = \prod_{j'=1}^R S(itp_{2m-1j'}) \quad (85)$$

with the 2-order symmetrized decomposition $S(it)$:

$$\begin{aligned} S(it) = & \exp[-itA_j(-M \times l, 0, \omega)/2] \dots \exp[-itA_j(M \times l, n-2, \omega)/2] \\ & \times \exp[-itA_j(M \times l, n-1, \omega)] \exp[-itA_j(M \times l, n-2, \omega)/2] \dots \\ & \times \exp[-itA_j(-M \times l, 0, \omega)/2] \end{aligned} \quad (86)$$

where the parameters $\{p_{2m-1j'}\}$ are normalized, $\sum_{j'=1}^R p_{2m-1j'} = 1$, and it has been shown that the $2m$ -order symmetrized decomposition really equals to the $(2m-1)$ -order one [39]. The explicit determination for the parameters $\{p_{2m-1j'}\}$ in Eq.(85) is given in Refs.[39, 40]. By exploiting the generalized Trotter-Suzuki formula [39, 40] one can obtain more accurate symmetrized decomposition with the smaller error of order $O(L^{-(2m-1)}t^{2m})$ from Eq.(84)

$$\begin{aligned} \exp\{-it \sum_{k'=0}^{n-1} \sum_{k=-M \times l}^{M \times l} A_j(k, k', \omega)\} = & [f_{2m-1}(\{\frac{1}{L}A_j(k, k', \omega)\})]^L \\ & + O(t^{2m}/L^{(2m-1)}). \end{aligned} \quad (87)$$

There are $[2n(2M \times l + 1) - 1]$ unitary operators $\exp[-itpA_j(k, k', \omega)]$ for each two-order symmetrized decomposition $S(it)$ of Eq.(86). Then there are $R[2n(2M \times l + 1) - 1]$ unitary operators $\exp[-itpA_j(k, k', \omega)]$ in the $(2m-1)$ -order symmetrized decomposition $f_{2m-1}(\{A_j(k, k', \omega)\})$ of Eq.(85) and the symmetrized decomposition of Eq.(87) contains the unitary operators with the total number of $LR[2n(2M \times l + 1) - 1]$.

Now inserting the symmetrized decomposition (87) into Eq.(79) the unitary operator $\exp(-i\theta a_j^s I_{jz})$ is expressed as

$$\begin{aligned} \exp(-i\theta a_j^s I_{jz}) = & [f_{2m-1}(\{\frac{1}{L}A_j(k, k', \omega)\})]^L [f_{2m-1}(\{\frac{1}{L}A_j(k, k', -\omega)\})]^L \\ & + O_0(M, l) + O(t^{2m}/L^{(2m-1)}). \end{aligned} \quad (88)$$

As the final result, the oracle unitary operation $U_{oz}(\theta)$ can be expressed as a

sequence of the unitary operations $\exp[-itpA_j(k, k', \omega)]$ which consist of the selective phase-shift operations and the nonselective unitary operations,

$$U_{oz}(\theta) = \prod_{j=1}^n \{ [f_{2m-1}(\{\frac{1}{L}A_j(k, k', \omega)\})]^L [f_{2m-1}(\{\frac{1}{L}A_j(k, k', -\omega)\})]^L \} \\ + nO_0(M, l) + nO(t^{2m}/L^{(2m-1)}). \quad (89)$$

It has been shown that the decomposition of Eq.(89) is much more accurate than that of Eq.(83) and thus, the number of the exponential unitary operations $\exp[-itpA_j(k, k', \omega)]$ in Eq.(89) is much less than that one in Eq.(83) with the same error in magnitude [39]. Now number of the selective phase-shift operations $C_s(\theta)$ to compose the oracle unitary operation $U_{oz}(\theta)$ can be evaluated from the expression (89). The oracle unitary operation $U_{oz}(\theta)$ contains $2nLR[2n(2M \times l + 1) - 1]$ unitary operations $\exp[-itpA_j(k, k', \omega)]$, whereas equations (46), (66), and (82) show that each unitary operation $\exp[-itpA_j(k, k', \omega)]$ contains four selective phase-shift operations $C_s(\theta)$. Therefore, the oracle unitary operation $U_{oz}(\theta)$ really consists of the number $8nLR[2n(2M \times l + 1) - 1]$ of the selective phase-shift operations $C_s(\theta)$ in addition to the nonselective unitary operations. On the other hand, it can be seen from Eqs.(46), (66), (80), (82)-(89) that all the nonselective unitary operations including $\exp(\pm i\pi F_y)$, $\exp(\pm i\frac{\pi}{2}F_{jy})$, $\exp(\pm i\varphi_{jk}F_{jz})$, and $\exp(\pm i2\pi \sum_{k=1, k \neq j}^n \varphi_k I_{kz})$, etc., (note that the index j runs over all n particles in the quantum system so that $\exp(\pm i\frac{\pi}{2}F_{jy})$, etc., become the nonselective unitary operations) in the oracle unitary operation $U_{oz}(\theta)$ are one-qubit unitary operations and the total number of these nonselective unitary operations is proportional to the number $nLR[2n(2M \times l + 1) - 1]$. Therefore, the oracle unitary operation $U_{oz}(\theta)$ can be really expressed explicitly as a sequence of the number $O(nLR[2n(2M \times l + 1) - 1])$ of the selective phase-shift operations $C_s(\theta)$ and the number $O(nLR[2n(2M \times l + 1) - 1])$ of the nonselective unitary operations. Obviously, the quantum network U_S of Eq.(34) with the oracle unitary operation (89) or (83) could be a polynomial-time quantum search network only when the lattice point number $(2M \times l + 1)$ of the numerical integration (65) does not increase exponentially as the dimensional size n of the multiple integral (63).

8. Discussion

As shown in previous sections, the multiple-quantum operator algebra formalism has been exploited to construct explicitly a real quantum search algorithm. In an unsorted search problem the initial state, i.e., the superpo-

sition, and the final state, that is, the target state, are usually given and fixed in a quantum system. Then the propagator and its corresponding effective Hamiltonian can be constructed explicitly that describe in quantum mechanics the time evolution of the quantum system from the initial state to the final of the search problem. A real quantum search algorithm could be built up by starting out such propagator, although the propagator may usually not be compatible with the mathematical structure and principle of the search problem and hence is not a real quantum search network. There are two families of elementary unitary operations, that is, the nonselective unitary operations and the oracle unitary operations, for example, the selective phase-shift operations, in the unsorted quantum search problem. These elementary unitary operations are compatible with the mathematical structure and principle of the search problem. Then, the propagator is compatible with the mathematical structure and principle of the search problem and becomes a real quantum search network when it is expressed explicitly as a sequence of the nonselective and the selective unitary operations. The multiple-quantum operator algebra formalism plays an important role in the general construction of the quantum search algorithm. In particular, the discrete Fourier analysis and the phase cycling technique based on the characteristic transformation behavior of multiple-quantum coherence operators under the z-axis rotations are very helpful for the construction of the quantum search networks.

An unsorted search problem in a large unsorted database is a hard problem in classical computation and there has not been any efficient classical search algorithm to solve the NP problem in polynomial time so far. Grover has showed that the search problem can be fast solved by a quadratically speed-up quantum search algorithm over any classical algorithms [14]. However, the Grover algorithm is not really a polynomial-time quantum search algorithm. In the paper two possible schemes are proposed to solve the unsorted search problem. One scheme is based on the NMR devices [24] (see Appendix A and C). The oracle unitary operations $U_{0p}(\theta)$ ($p = x, y, z$) in the quantum network U_S of Eq.(34) could be implemented directly on the NMR devices and hence the quantum network U_S becomes a real unsorted quantum search network. With the help of the NMR device [24] the unsorted search problem which is an NP-problem is converted into a special knapsack problem which can be solved efficiently in polynomial time (see Appendix A), indicating that the unsorted search problem could be solved efficiently on the NMR quantum computer in polynomial time. Another is that the oracle unitary operations $U_{0p}(\theta)$ are expressed as a sequence of the nonselective

unitary operations and the selective phase-shift operations which can be implemented directly on an oracle universal quantum computer with the help of the phase cycling technique, the numerical multidimensional integration and the Trotter-Suzuki theory. It has been shown that the computational complexity of the unsorted quantum search algorithm is dependent mainly upon that of the numerical multidimensional integration. The proper numerical multidimensional integration methods should satisfy the requirement that the lattice point number to numerically integrate the multidimensional integral (63) does not increase exponentially as the dimensional size of the multiple integral within the desired error so that the constructed quantum search algorithm becomes an efficient algorithm. One of the possible numerical methods of multiple integration [30-37] to evaluate the multiple integral (63) may be the Hua-Wang number-theoretic method [31, 32]. It is believed that with the Hua-Wang method the lattice point number of numerical integration does not increase exponentially as the dimensional size of the multiple integral (63). As a consequence, it is believed that the quantum network U_S of Eq.(34) could be an efficient quantum search network on an oracle universal quantum computer. Therefore, it is believed that quantum computers could solve efficiently a general NP-problem in polynomial time.

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Appendix A

An NMR model based on the spectral labeling [24] is proposed to solve efficiently the unsorted search problem experimentally. It is based on the massive parallelism of quantum computation and the noncollapse, nonde-molition, and phase-sensitive measurement in NMR techniques. This NMR model could offer the possibility to transform the hard NP-problem of the unsorted search problem into the polynomial-time problem, resulting in that the hard problem could be solved efficiently. This result supports the belief that a quantum computer could solve in principle a general NP-problem, although the present model could work only on a few-qubit system. The spectral labeling on the NMR quantum computing is first proposed by Madi, Bruschweiler, and Ernst [24]. One of the advantages of the method over the

other state labelings is that each resonance peak of the NMR spectrum of the ancillary spin corresponds one-to-one to a quantum state of the work space of quantum computation. This labeling method requires that the ancillary spin be coupled with all the spins in the work space and all single-quantum transitions of the ancillary spin be nondegenerate. This may limit the practical application of the model in an NMR system with many qubits. However, it provides a very simple experiment model to solve efficiently the unsorted search problem.

Consider the weakly coupled spin ($I=1/2$) system SAMX... as a quantum computation device, that is, an NMR quantum computer. The spin S is the ancillary qubit and the spins A, M, X, \dots form the work space of the quantum computation. In particular, assume that all the spins A, M, X, \dots couple with the spin S . In order to exploit the massive parallelism of quantum computation the system is first prepared at a superposition including the marked state $|s\rangle$:

$$|\Psi\rangle = |r, S\rangle = \sum_{x=0}^{N-1} a_x |x\rangle [\frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)]$$

where the ancillary qubit S is at the superposition $\frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)$. The evaluation of the function $f(x)$ then can be achieved by performing the oracle unitary operation U_f on the superposition

$$\begin{aligned} U_f : |\Psi\rangle &\rightarrow \sum_{x=0}^{N-1} a_x |x\rangle [\frac{1}{\sqrt{2}}(|0 \oplus f(x)\rangle - |1 \oplus f(x)\rangle)] \\ &= \sum_{x=0, x \neq s}^{N-1} a_x |x\rangle [\frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)] - a_s |s\rangle [\frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)] \end{aligned}$$

where it has been introduced the fact that the function $f(s) = 1$ and $f(r) = 0$, $r \neq s$. Obviously, only the target state $|s\rangle [\frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)]$ is inverted and any other states keep unchanged when performing each evaluation of the function $f(x)$. In general, it is difficult to distinguish the inverted target state from the other states in a quantum system after performing only once evaluation of the function $f(x)$. This is because each state has the equal probability. However, there is a significant phase difference between the target state and any other state after implementing once evaluation of the function $f(x)$. The phase of the target state is opposite to all of the other states. In the Grover quantum search algorithm [14] this phase difference is transferred into an amplitude difference between the target state and the other states by making the diffusion transformation so that the amplitude of the target state is amplified, resulting in that the search is quadratically speeded up. It is well-known that the phase difference among states in a nuclear spin ensemble

may be detected by the nuclear magnetic resonance (NMR) measurement techniques. The NMR signals and spectra carry the information of the phase difference. Now, it is possible to reveal the effect of the phase difference on the NMR spin ensemble, and especially on the phase and amplitude of the NMR spectra if the evaluation of the function $f(x)$ is performed on an NMR quantum computer. This phase difference may result in the phase-inversion spectrum of the target state with respect to those peaks of the other states. As an example, Figure One (see central spectrum) is the conventional NMR spectrum of the ancillary spin S in a four-qubit spin system SAMX. When the evaluation of the function $f(s)$ ($|s\rangle = |\alpha\beta\beta\rangle$) is carried out the target state $|\alpha\beta\beta\rangle|S\rangle$ is inverted in phase. Now, if the NMR spectrum of the ancillary qubit S is recorded one may find the phase-inversion peak of the target state (see bottom spectrum). It shows how the resonant peak of the target state with inversion phase may be recognized from the others peaks. The resonant frequency of the phase-inversion peak can be measured accurately if the signal-to-noise ratio of the peak is high enough. The resonant frequency actually carries some information of the target state. It is expected to extract the information from the resonant frequency.

The spin Hamiltonian of the weakly coupled spin ($I=1/2$) system SAMX... can be written generally as

$$H = \Omega_S S_z + \sum_{k=1}^n \Omega_k I_{kz} + S_z \sum_{k=1}^n J_{Sk} I_{kz} + \sum_{l>k=1}^n J_{kl} I_{kz} I_{lz} \quad (A1)$$

where the contribution of the decoherence has been neglected; the symbol I denotes the spins A, M, X, ..., and Ω_S , Ω_k are the chemical shifts of the spin S and the k th spin I , respectively; J_{Sk} is the scalar coupling constant between the spin S and the k th spin I , J_{kl} the scalar coupling constant of the k th and the l th spin I . Obviously, the conventional quantum computational base $|r, S\rangle = |r\rangle|S\rangle$ are the eigenbase of the spin Hamiltonian (A1) with the corresponding energy eigenvalue $E(r, S)$,

$$H|r\rangle|S\rangle = E(r, S)|r\rangle|S\rangle,$$

$$E(r, S) = \frac{1}{2}b_S(\Omega_S + \sum_{k=1}^n \frac{1}{2}a_k^r J_{Sk}) + \sum_{k=1}^n \frac{1}{2}a_k^r \Omega_k + \sum_{l>k=1}^n \frac{1}{4}a_k^r a_l^r J_{kl} \quad (A2)$$

where the unity-number representation of the eigenbase $|r, S\rangle$ has been used (see Eq.(18)),

$$|r, S\rangle = (\frac{1}{2}T_1 + a_1^r S_1) \otimes (\frac{1}{2}T_2 + a_2^r S_2) \otimes \dots \otimes (\frac{1}{2}T_n + a_n^r S_n) \otimes (\frac{1}{2}T_S + b_S S_S).$$

For an arbitrary computational basis $|r\rangle$ of spins I the transition frequency of the ancillary spin S is written as

$$\omega_S(r) = E(r, S = +1/2) - E(r, S = -1/2) = \Omega_S + \sum_{k=1}^n \frac{1}{2}a_k^r J_{Sk}. \quad (A3)$$

The scalar coupling constants J_{Sk} and the chemical shift Ω_S are usually fixed for a given weakly coupled spin system. If one can measure exactly the resonant frequency $\omega_S(r)$ in an NMR experiment the unity-number vector $\{a_k^r\}$ will be determined from the above equation (A3) which can be reduced to the form

$$\sum_{k=1}^n b_k^r J_{Sk} = f_S(r) \quad (A4)$$

where $b_k^r = \frac{1}{2}(a_k^r + 1) = 0, 1; k = 1, 2, \dots, n$ and $f_S(r) = \omega_S(r) - \Omega_S + \sum_{k=1}^n \frac{1}{2} J_{Sk}$. Obviously, it is the famous knapsack problem to solve exactly equation (A4). It is well known that the knapsack problem is generally an NP-complete problem [42, 43]. Then it is usually hard to solve equation (A4). The degree of difficulty of the problem (A4) is crucially dependent upon the choice of the coefficients of Eq.(A4), i.e., the scalar coupling constants $\{J_{Sk}\}$. For example, if the scalar coupling constant set $\{J_{Sk}, k = 1, 2, \dots, n\}$ is a superascend sequence, that is, $J_{Sk} > 0$ ($k = 1, 2, \dots, n$) and

$$J_{Sk+1} > \sum_{l=1}^k J_{Sl}, \quad (1 \leq k < n-1),$$

equation (A4) can be solved efficiently in polynomial time [42, 43]. Once the unity number vector $\{a_k^s\}$ is determined, the oracle unitary operation $U_{op}(\theta) = \prod_{k=1}^n \exp[-i\theta a_k^s I_{kp}]$ can be directly implemented experimentally on a universal quantum computer. Then the target state $|s\rangle$ can be obtained by making directly the quantum search network U_S of Eq.(34) on the superposition $|\Psi\rangle$ in Eq.(19). It must be pointed out that there are a number of choices of the coefficients in Eq.(A4) besides the above superascend sequence so that equation (A4) can be solved efficiently in polynomial time [42-44].

The above NMR model [24] transforms really the NP-problem, i.e., the unsorted quantum search problem, to the polynomial-time problem, i.e., the special knapsack problem [42, 43].

Caption of Figure 1. A simple NMR device with the weakly coupled four-spin ($I=1/2$) system SAMX to solve efficiently the unsorted search problem. The spin S acts as the auxiliary qubit. Note that the peak of the target state $|\alpha\beta\beta\rangle|S\rangle$ is inverted in phase with respect to other peaks, as can be seen in bottom spectrum.

Appendix B

If the multidimensional function $f(x_1, x_2, \dots, x_n)$ can be expanded as the absolutely convergent Fourier series:

$$f(x_1, x_2, \dots, x_n) = \sum_{m_1, \dots, m_n = -\infty}^{\infty} C(m_1, m_2, \dots, m_n) \times \exp[-i2\pi(m_1x_1 + m_2x_2 + \dots + m_nx_n)] \quad (B1)$$

with the complex expansion coefficients $C(m_1, m_2, \dots, m_n)$ and integer indexes $\{m_k; k = 1, 2, \dots, n\}$, and if the integer weight functions $\Phi(M, l, j)$ are defined by the following identity

$$\left(\sum_{j=-M}^M Z^j \right)^l = \sum_{j=-M \times l}^{M \times l} \Phi(M, l, j) Z^j, \quad (B2)$$

then one has the numerical multiple integration formula:

$$\begin{aligned} & \int_0^1 \dots \int_0^1 dx_1 \dots dx_n f(x_1, x_2, \dots, x_n) \\ &= \frac{1}{(2M+1)^l} \sum_{j=-M \times l}^{M \times l} \Phi(M, l, j) f(j\boldsymbol{\omega}) + O(M, l) \end{aligned} \quad (B3)$$

with the n -dimensional real algebraic number lattice point $\boldsymbol{\omega} = (\omega_1, \omega_2, \dots, \omega_n)$, and the error function operator $O(M, l)$ can be expressed as

$$O(M, l) = - \sum'_{m_1, \dots, m_n = -\infty}^{\infty} C(m_1, m_2, \dots, m_n) \left(\frac{\sin[(2M+1)\pi(\mathbf{m}, \boldsymbol{\omega})]}{(2M+1)\sin[\pi(\mathbf{m}, \boldsymbol{\omega})]} \right)^l \quad (B4)$$

where the sums \sum' with the prime symbol do not include the term with $m_1 = m_2 = \dots = m_n = 0$ and the dot product $(\mathbf{m}, \boldsymbol{\omega}) = m_1\omega_1 + m_2\omega_2 + \dots + m_n\omega_n$.

Proof: The detailed proof for the above theorem can be seen in references [31, 32]. Note that the multiple integral on the left-hand side of Eq.(B3) equals the coefficient $C(m_1, m_2, \dots, m_n)$ with $m_1 = m_2 = \dots = m_n = 0$,

$$C(0, 0, \dots, 0) = \int_0^1 \dots \int_0^1 dx_1 \dots dx_n f(x_1, x_2, \dots, x_n).$$

Because the Fourier series of Eq.(B1) is absolutely convergent one has

$$\begin{aligned} & \frac{1}{(2M+1)^l} \sum_{j=-M \times l}^{M \times l} \Phi(M, l, j) f(j\boldsymbol{\omega}) = \frac{1}{(2M+1)^l} \sum_{m_1, \dots, m_n = -\infty}^{\infty} C(m_1, m_2, \dots, m_n) \\ & \quad \times \sum_{j=-M \times l}^{M \times l} \Phi(M, l, j) \exp[-i2\pi j(m_1\omega_1 + m_2\omega_2 + \dots + m_n\omega_n)] \\ &= C(0, 0, \dots, 0) + \frac{1}{(2M+1)^l} \sum'_{m_1, \dots, m_n = -\infty}^{\infty} C(m_1, m_2, \dots, m_n) \\ & \quad \times \left(\sum_{j=-M}^M \exp[-i2\pi j(m_1\omega_1 + m_2\omega_2 + \dots + m_n\omega_n)] \right)^l \\ &= \int_0^1 \dots \int_0^1 dx_1 \dots dx_n f(x_1, x_2, \dots, x_n) \end{aligned}$$

$$+ \sum_{m_1, \dots, m_n = -\infty}^{\infty} C(m_1, m_2, \dots, m_n) \left(\frac{\sin[(2M+1)\pi(\mathbf{m}, \boldsymbol{\omega})]}{(2M+1) \sin[\pi(\mathbf{m}, \boldsymbol{\omega})]} \right)^l$$

where the identity (B2) has been introduced. Obviously, if the error function $O(M, l)$ is given by Eq.(B4) then the numerical integration formula (B3) is obtained.

To calculate explicitly the error function operator $O(M, l)$ in the numerical integration (65) the integrand operator (66) of the multiple integral (63) is first expanded under any pair of the usual computational bases $|r\rangle$ and $|t\rangle$ and the corresponding matrix element then is written as

$$\langle r | G_{jq}(y_1, y_2, \dots, y_n) | t \rangle = \langle r | \theta H_{jq} | t \rangle \exp[-i2\pi \sum_{k=1, k \neq j}^n m_k(r, t) y_k] \quad (B5)$$

where the integer vector $\mathbf{m} = \{m_k(r, t)\}$ with $m_k(r, t) = -1, 0, +1$; $k = 1, 2, \dots, n$ for any pair of bases $|r\rangle$ and $|t\rangle$, and $m_1(r, t) = m_2(r, t) = \dots = m_n(r, t) = 0$ when $|r\rangle = |t\rangle$. Then, the error function operator $O(M, l)$ in the numerical integration (65) with the integrand (B5) can be found from Eq.(B4),

$$\langle r | O(M, l) | t \rangle = -\langle r | \theta H_{jq} | t \rangle \left(\frac{\sin[(2M+1)\pi(\mathbf{m}, \boldsymbol{\omega})]}{(2M+1) \sin[\pi(\mathbf{m}, \boldsymbol{\omega})]} \right)^l \quad (r \neq t).$$

Obviously, $\langle r | O(M, l) | t \rangle = 0$ for any pair of bases $|r\rangle = |t\rangle$.

Appendix C

In appendix A the NMR device [24] is used to measure experimentally the unity-number vector $\{a_k^s\}$ in polynomial time. However, this device is quite limited in practice. Therefore, one hopes naturally that there is a convenient NMR device to measure efficiently the unity-number vector. It had better start at the thermal equilibrium state of an NMR quantum ensemble instead of the effective pure state [46]. That is, this NMR device can exploit the initial mix state of a spin system, for example, the thermal equilibrium state to determine experimentally the unity-number vector and hence it may be useful in practice. The present device is still based on the massive parallelism of quantum computation and the phase-sensitive NMR measurement.

In section 4 it has been shown that the selective phase-shift operation $C_s(\theta)$ can be equivalent to the oracle unitary operation U_f when the auxiliary qubits are used in the implementation of the quantum search problem. For example, $C_s(\pi) = U_f$ (equivalent) when the auxiliary qubit S takes the superposition $|S\rangle = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)$ in the superposition:

$$|\Psi_1\rangle = |I, S\rangle = \sum_{x=0}^{N-1} a_x |x\rangle [\frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)] \quad (C1)$$

where the selective phase-shift operation $C_s(\pi)$ is applied only to the work qubits I , while the oracle unitary operation U_f , that is, the evaluation of function $f(s)$, is applied to all the qubits including both the work qubits I and the auxiliary qubit S . It is also shown that the selective phase-shift operation $C_s(\theta)$ can be expressed as $C_s(\theta) = U_f V(\theta) U_f$ (equivalent) on the superposition:

$$|\Psi_2\rangle = |I, S\rangle = \sum_{x=0}^{N-1} a_x |x\rangle |0\rangle |1\rangle \quad (C2)$$

where the state of the auxiliary qubits S takes $|S\rangle = |0\rangle |1\rangle$. On the other hand, in the matrix representation the superposition (C1) and (C2) can be expressed respectively as

$$\rho_1 = |\Psi_1\rangle\langle\Psi_1| = \rho_{1I} \otimes \rho_{1S} \quad (C3)$$

with $\rho_{1I} = (\sum_{x,y=0}^{N-1} a_x a_y |x\rangle\langle y|)$ and $\rho_{1S} = \frac{1}{2}(|0\rangle - |1\rangle)(-\langle 1| + \langle 0|)$, and

$$\rho_2 = |\Psi_2\rangle\langle\Psi_2| = \rho_{2I} \otimes \rho_{2S} \quad (C4)$$

with $\rho_{2I} = (\sum_{x,y=0}^{N-1} a_x a_y |x\rangle\langle y|)$ and $\rho_{2S} = |0\rangle\langle 0| \otimes |1\rangle\langle 1|$. Then there are the following relations when the oracle unitary operations U_f and $U_f V(\theta) U_f$ applied to the two superpositions (C3) and (C4), respectively,

$$U_f \rho_1 U_f^{-1} = C_s(\pi) \rho_{1I} C_s(\pi)^{-1} \otimes \rho_{1S}, \quad (C5)$$

$$U_f V(\theta) U_f \rho_2 (U_f V(\theta) U_f)^{-1} = C_s(\theta) \rho_{2I} C_s(\theta)^{-1} \otimes \rho_{2S} \quad (C6)$$

This shows that the action of the selective phase-shift operations $C_s(\theta)$ and $C_s(\pi)$ on the work qubits I is equivalent to the action of the oracle unitary operations $U_f V(\theta) U_f$ and U_f on the whole system including the auxiliary qubits S , respectively. Although the density operators ρ_1 and ρ_2 are pure states in Eqs.(C5) and (C6), the two equations (C5) and (C6) still hold even when the density operators ρ_{1I} and ρ_{2I} take any mix states of the work qubits I . This is because the unitary operations U_f , $V(\theta)$, and $C_s(\theta)$ are linear operators. Then the equivalent relations: $C_s(\pi) = U_f$ and $C_s(\theta) = U_f V(\theta) U_f$ still hold even when the density operators ρ_{1I} and ρ_{2I} are taken as the mix states of the work qubits I in Eqs.(C5) and (C6). This point is important for the NMR experimental determination for the unity-number vector $\{a_k^s\}$ by starting out the mix state ρ_{1I} or ρ_{2I} of the work qubits I , e.g., the thermal equilibrium state, instead of the effective pure state.

In NMR experiments to determine the unity-number vector $\{a_k^s\}$ the density operators ρ_{1I} and ρ_{2I} may be prepared as any mix states of the work

qubits I , but the auxiliary qubits S must be prepared as the effective pure states ρ_{1S} and ρ_{2S} , respectively. On the other hand, if the density operators ρ_{1I} and ρ_{2I} do not include the marked state $|s\rangle$ one has

$$C_s(\pi)\rho_{1I}C_s(\pi)^{-1} = \rho_{1I}, \quad C_s(\theta)\rho_{2I}C_s(\theta)^{-1} = \rho_{2I}.$$

In this case it is impossible to determine experimentally the unity-number vector $\{a_k^s\}$. Thus, it is required that the density operators ρ_{1I} and ρ_{2I} be taken as any mix state that include any given marked state $|s\rangle$. As a simple example, the density operator (ρ_{1I} or ρ_{2I}) including any given marked state $|s\rangle$ may be taken as

$$\rho_I = \alpha_0 E + \sum_{k=1}^n \varepsilon_k I_{k\mu} \quad (\mu = x, y) \quad (C7)$$

This density operator can be generated from the thermal equilibrium state of the work qubits: $\rho_{0I} = \alpha_0 E + \sum_{k=1}^n \varepsilon_k I_{kz}$ by applying a ninety degree pulse.

It is assumed in the following discussion that the auxiliary qubits S are always prepared as the effective pure states ρ_{1S} and ρ_{2S} , respectively, during the action of the oracle unitary operations U_f and $U_f V(\theta) U_f$ so that the two oracle unitary operations can be replaced by their corresponding selective phase-shift operations $C_s(\pi)$ and $C_s(\theta)$, respectively, to describe the evolution process during the oracle unitary operation

$$\rho_{1S} = (\frac{1}{2}|0\rangle\langle 0| + \frac{1}{2}|1\rangle\langle 1| - \frac{1}{2}|0\rangle\langle 1| - \frac{1}{2}|1\rangle\langle 0|) = \frac{1}{2}E - S_x, \quad (C8)$$

$$\begin{aligned} \rho_{2S} &= |0\rangle\langle 0| \otimes |1\rangle\langle 1| = (\frac{1}{2}E_1 + S_{1z}) \otimes (\frac{1}{2}E_2 - S_{2z}) \\ &= \frac{1}{4}E + \frac{1}{2}(S_{1z} - S_{2z}) - S_{1z}S_{2z} \end{aligned} \quad (C9)$$

In order to analyse the evolution process during the oracle unitary operation the selective phase-shift operation $C_s(\theta)$ is decomposed into a sequence of elementary propagators built up with the base operators of the *LOMSO* operator subspace [18,19]

$$\begin{aligned} C_s(\theta) &= \exp(-i\theta_s^*) \exp[-i\theta_s^* (\sum_{k=1}^n a_k^s 2I_{kz})] \exp[-i\theta_s^* (\sum_{l>k=1}^n a_k^s a_l^s 4I_{kz}I_{lz})] \\ &\times \exp[-i\theta_s^* (\sum_{l>k=1}^n a_k^s a_l^s a_m^s 8I_{kz}I_{lz}I_{mz})] \dots \end{aligned} \quad (C10)$$

where $\theta_s^* = \theta_s/N$. Then it is easy to prove that there are the basic unitary transformation relations for the oracle unitary operation

$$\begin{aligned} C_s(\theta)I_{kx}C_s(\theta)^{-1} &= I_{kx} \cos[\theta_s^* \cdot 2(E + \sum_{l=1}^n a_l^s 2I_{lz} + \sum_{m>l=1}^n a_l^s a_m^s 4I_{lz}I_{mz} + \dots)] \\ &+ a_k^s I_{ky} \sin[\theta_s^* \cdot 2(E + \sum_{l=1}^n a_l^s 2I_{lz} + \sum_{m>l=1}^n a_l^s a_m^s 4I_{lz}I_{mz} + \dots)] \end{aligned} \quad (C11a)$$

$$C_s(\theta)I_{ky}C_s(\theta)^{-1} = I_{ky} \cos[\theta_s^*.2(E + \sum_{l=1}^n a_l^s 2I_{lz} + \sum_{m>l=1}^n a_l^s a_m^s 4I_{lz}I_{mz} + \dots)] \\ - a_k^s I_{kx} \sin[\theta_s^*.2(E + \sum_{l=1}^n a_l^s 2I_{lz} + \sum_{m>l=1}^n a_l^s a_m^s 4I_{lz}I_{mz} + \dots)] \quad (C11b)$$

where the sums \sum' run over all indexes except the index k . To simplify further the unitary transformation relations (C11a) and (C11b) the triangular functions of the *LOMSO* operator subspace are expanded in terms of the *LOMSO* base operators [18]

$$\cos[\theta_s^*.2(E + \sum_{l=1}^n a_l^s 2I_{lz} + \sum_{m>l=1}^n a_l^s a_m^s 4I_{lz}I_{mz} + \dots)] = \alpha'_{0k} E + \sum_{l=1}^n \Omega'_{kl} I_{lz} \\ + \sum_{m>l=1}^n J'_{klm} 2I_{lz}I_{mz} + \sum_{p>m>l=1}^n J'_{klmp} 4I_{lz}I_{mz}I_{pz} + \dots \quad (C12a)$$

$$\sin[\theta_s^*.2(E + \sum_{l=1}^n a_l^s 2I_{lz} + \sum_{m>l=1}^n a_l^s a_m^s 4I_{lz}I_{mz} + \dots)] = \alpha''_{0k} E + \sum_{l=1}^n \Omega''_{kl} I_{lz} \\ + \sum_{m>l=1}^n J''_{klm} 2I_{lz}I_{mz} + \sum_{p>m>l=1}^n J''_{klmp} 4I_{lz}I_{mz}I_{pz} + \dots \quad (C12b)$$

Now start the initial state ρ_I (C7) ($\mu = x$). By applying the oracle unitary operation and then a hard 90_x° pulse to the spins I the state is transferred into

$$\rho_f = R(90_x)C_s(\theta)\rho_I C_s(\theta)^{-1}R(90_x)^{-1} \otimes \rho_{2S} \\ = \alpha_0 E \otimes \rho_{2S} + \sum_{k=1}^n \varepsilon_k I_{kx} \{ \alpha'_{0k} + \sum_{l=1}^n \Omega'_{kl} (-I_{ly}) \\ + \sum_{m>l=1}^n J'_{klm} 2I_{ly}I_{my} + \sum_{p>m>l=1}^n J'_{klmp} 4(-I_{ly}I_{my}I_{py}) + \dots \} \otimes \rho_{2S} \\ + \sum_{k=1}^n \varepsilon_k a_k^s I_{kz} \{ \alpha''_{0k} E + \sum_{l=1}^n \Omega''_{kl} (-I_{ly}) + \sum_{m>l=1}^n J''_{klm} 2I_{ly}I_{my} \\ + \sum_{p>m>l=1}^n J''_{klmp} 4(-I_{ly}I_{my}I_{py}) + \dots \} \otimes \rho_{2S} \quad (C13)$$

This state is quite inconvenient for the NMR measurement of the unity-number vector $\{a_k^s\}$. However, by applying a purge pulse unit [47] such as z-direction gradient field, z-filter, etc., on the density operator (C13) to cancel all the multiple-quantum coherences including the zero-quantum coherences but leave only the longitudinal magnetization and spin order components unchanged, the density operator (C13) is reduced to the form

$$\rho_f = \{ \alpha_0 E + \sum_{k=1}^n \alpha''_{0k} \varepsilon_k a_k^s I_{kz} \} \otimes \rho_{2S} \quad (C14)$$

The parameters $\{\alpha''_{0k}\}$ can be obtained explicitly from Eq.(C12b),

$$\alpha''_{0k} = \frac{2}{N} \sum'_{m_i, m_p, m_q, \dots} \sin\left\{ \frac{2}{N} \theta_s [1 + \sum_{i=1}^n a_i^s 2m_i + \sum_{p>i=1}^n a_i^s a_p^s 4m_i m_p + \dots] \right\} \quad (C15)$$

where $m_i, m_p, m_q, \dots = 1/2, -1/2$ and the sums \sum' run over all indexes except the index m_k . It turns out that the parameters $\alpha''_{0k} = 1/2^{n-1}$ when the phase angle $\theta_s = \pi/2$. Now the density operator ρ_f of Eq.(C14) is quite simple. The unity-number vector $\{a_k^s\}$ can be measured simply from the state of Eq.(C14). The measurement may be carried out conveniently by applying a hard 90_y° pulse to the spins I of the density operator of Eq.(C14) and then recording the NMR signal of the spins I during decoupling the auxiliary spins S . Obviously, the unity-number vector $\{a_k^s\}$ may be determined conveniently by recording and comparing both two NMR spectra of the density operators (C7) and (C14), respectively.

With respect to the NMR device in Appendix A the present NMR device can be even a spin ensemble of linear molecules with neighbor interaction and moreover, the auxiliary spins in the device are not required to interact with all spins of the work qubits. Therefore, the present NMR device is very convenient one to determine the unity-number vector and may be more useful in practice. However, the NMR signal of the spins I of the density operator (C14) is proportional to $1/2^{n-1}$, indicating that it decreases exponentially as the I-spin number n . Thus, the main drawback of this device is that the NMR signal to determine sufficiently the unity-number vector $\{a_k^s\}$ decreases exponentially as the qubit number of the search problem. This is similar to the NMR quantum computing based on the effective pure state [48].

Although the NMR signal of the density operator (C14) decreases exponentially as the qubit number n like the NMR quantum computing on the effective pure state, it must be pointed out that they have a significant difference. The present device can start at the thermal equilibrium state of spin ensemble, while the latter starts at the effective pure state [46, 49]. The present scheme to measure the unity-number vector is polynomial-time within the realizable size of NMR quantum computation, but the Grover algorithm based on the pure quantum state [14] or the effective pure state [49] is a quadratically speed-up method even within the realizable size of NMR technique. Although in the present NMR device the final NMR signal of Eq.(C14) may not be detected due to too low signal-to-noise ratio in a spin system with many qubits, this is the NMR *technique limit* instead of the *principle limit*. Therefore, the final result $\{a_k^s\}$ will be obtained certainly in polynomial time if the sensitivity of the NMR signal of Eq.(C14) is improved sufficiently in NMR technique [46]. However, in the version of the Grover algorithm based on the pure quantum state [14] or the effective pure state [49] each quantum state in the superposition has the same probability,

then the marked state in the superposition is impossible to be found certainly after performing once the oracle unitary operation, i.e., the selective phase-shift operation, due to the limit of the quantum measurement principle [12] even when the measured signal sensitivity is increased sufficiently. One method to find certainly the marked state is to amplify the probability of the marked state but suppress all the others. This is just the spirit of the Grover algorithm [14].

There is an interesting thing. Suppose that the NMR signal of the density operator (C14) could be enhanced by applying a sequence of a polynomial number of the oracle unitary operations and the nonselective unitary operations on the initial state (C7), the realizable size of the present NMR device could be enlarged.